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ABSTRACT

Presented are some computer programs for undergraduate students. These computer programs were designed for use in standard chemical engineering courses such as kinetics, control, thermodynamics, transport, stagewise operation, and stoichiometry. Each of the 17 computer programs is presented in a separate section. Each section presents problem identification, technical description, educational aspects, and a program description. A summary for each of the 17 computer programs includes program title, author, cognizant supervisor, organization name, abstract, related programs, and program development information. (HM)

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(EN)

COMPUTER PROGRAMS FOR CHEMICAL ENGINEERING EDUCATION

CACHE

STAGEWISE COMPUTATIONS

C310, T.O.196

J. Christensen, University of Oklahoma, Editor

September 1972

U.S. DEPARTMENT OF HEALTH, EDUCATION & WELFARE
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COMPUTER PROGRAMS
for
CHEMICAL ENGINEERING

VOLUME VI - STAGEWISE OPERATIONS
James H. Christensen, University of Oklahoma, Editor

1973 National Academy of Engineering
Prepared under sponsorship of the National Science Foundation

This book is available at $6.00 per copy from Ernest J. Henley,
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Preface

A survey of American chemical engineering departments conducted by the CACHE Committee in 1969 revealed that less than 25% of the basic chemical engineering courses had any computer content whatsoever. Relatively few transport, stoichiometry or thermodynamics courses made use of libray routines or required students to write programs. The incidence of computer usage was somewhat higher in the stagewise design and control courses.

One of the reasons computers are being neglected is that very few of the currently available chemical engineering textbooks contain either computer-oriented homework or example problems. It is unlikely that this situation will improve in the near future. The effort and expenses of developing and printing computer programs, and the limited chemical engineering market make it improblble that the badly needed computer oriented teaching aids can be made available through normal author-publisher channels.

Having established a need, the CACHE Committee, in March of 1971, voted to sponsor the collection and dissemination of sets of computer programs suitable for undergraduate courses. The concept was outlined in a memorandum submitted to CACHE by the curriculum subcommittee:

"The focus will be on small programs (rather than systems and packages). The programs should be suitable for use in 'standard' undergraduate courses; i.e. kinetics, control, thermodynamics, transport, stagewise operation, and stoichiometry.

"The programs should be well documented, debugged, and reasonably short (suitable as homework assignments). Standards and guidelines for 'approved' programs will be developed by the CACHE Standards Committee. Invitations to submit programs will be issued to all chemical engineering educators and an honorarium of $50 will be awarded for each program accepted.

"One editor will be put in charge of each course area, and he will work autonomously:

Kinetics - M. Reilly, Carnegie Mellon University
Thermodynamics - R. Jelinek, Syracuse University
Stoichiometry - E. Henley, University of Houston
Stagewise Computations - J. Christensen, University of Oklahoma
Transport - R. Gordon, University of Florida
Design - R. Jelinek, University of Syracuse
Control - A. Westerberg, University of Florida

The response to the invitations to submit programs was much greater than had been anticipated. More than five hundred excellent program abstracts were submitted, and the budget precluded publishing more than one hundred. As an Appendix to most of these volumes we list some of the programs we were not able to accommodate because of lack of space and funds.

We hope that we, as editors, have chosen wisely and that chemical educators throughout the world will benefit from the ideas and experience embodied in these volumes. We are grateful for the cooperation and the diligence of the authors and we commend their efforts to the readers.

Ernest J. Henley
Houston, Texas 1972

Foreword

The problems in this volume represent a wide range of levels of complexity and of required student sophistication, from elementary stoichiometry through advanced thermodynamics and numerical methods. Accordingly, I have tried to arrange them in roughly the order in which they might be presented in a typical chemical engineering curriculum.

All of the programs submitted were compiled and run in the 110K byte student WATFIV batch partition of the University of Oklahoma's System 360/50 computer (except for problems 4, 16, and 17, which were too large to execute in this partition). The required storage and processor times, as well as total billing, for the examples shown in each problem writeup, are given in the table below. This procedure greatly facilitated the detection of non-ASA standard FORTRAN errors. Hence, I strongly recommend that any author desiring easy interchangeability of his programs submit them to a WATFOR or WATFIV compilation.

WATFIV COMPILATION RESULTS

	Storage (bytes)		Time (sec.)		Charge
program #	Program	Arrays	Compile	Run	
1	9,288	1440	2.22	17.62	-
2	4,344	0	1.57	2.14	-
3	7,832	248	1.49	1.29	
4	--	--	--	--	-
5	13,848	540	5.15	4.38	-
6	13,320	2500	3.24	9.32	-
7	7,472	804	3.57	60 (14/24 steps)	
8	7,824	800	2.77	2.29	-
9	13,552	3200	5.07	12.80	-
10	5,024	9040	6.60	2.82	$ 0.37
11	12,992	4612	7.03	17.53	1.57
12	11,704	400	2.74	7.61	0.88
13	14,200	724	4.02	7.92	0.83
14	18,792	2024	5.53	37.40	1.99
15	12,168	9688	4.68	60.01	3.14
			(run #1 only)		
16	740,352		11.37	--	1.09
			(compile only)		
17	32,712	128,864	9.65	--	0.93
			(compile only)		

Since many of the programs presented here are student efforts, it is to be expected that considerable inefficiency in use of storage and run time may be encountered in using many of the programs. However, I believe that one of the problem authors speaks for the majority, including myself, in saying: "I think it is rather important for the student to program the solution himself rather than to use canned routines." Thus, I hope that the programs listed here will be taken as points of departure for further improvement rather than as paragons of efficiency. In fact, I have had an enjoyable summer with an advanced projects course in improving the efficiency of several of these programs.

I would like to express my thanks to the editor of this series, Dr. E.J. Henley, for his patience, and to the many students who assisted me in program compilation and debugging, especially Mr. Chang-Ou Lee and Mr. Ching-Se Yen.

James H. Christensen
Norman, Oklahoma
July 24, 1973

I. PROBLEM IDENTIFICATION

1. Title: Stagewise Leaching Process Calculations
2. Author: Harry G. Folster
3. Affiliation: New Mexico State University

II. TECHNICAL DESCRIPTION

1. Problem Statement: The solution of extraction problems involve stage by stage calculations and as such are most easily solved by graphical techniques or by computer techniques. The use of a computer to perform the arithmetical calculations initially will involve more effort than finding solutions by graphical means. However, if the computer program is made sufficiently general, the overall result will be a savings in calculational time as compared to the graphical solutions if many extraction problems have to be solved. This is particularly true if the number of stages are fixed and trial and error calculations are required to determine one of the fresh feed rates to obtain a desired separation.

Write a computer program for determining the number of theoretical stages necessary to obtain the desired recovery of solute in a leaching process and test the program with the following problem:

> Copper sulfate in roasted ore is leached out with water in a continuous countercurrent extraction cascade. 100 tons/day of the ore containing 9.5 per cent $CuSO_4$, 85.5 per cent gangue, and 5 per cent moisture is contacted with water. The strong extract solution is to contain 10 per cent $CuSO_4$ and 90 per cent water. Since $CuSO_4$ is the valuable constituent, 97 per cent of it must be recovered in the extract. Experimental work has shown the gangue to retain 1.5 tons of water per ton of gangue.

A graphical solution should also be performed and the results compared to the computer solution.

2. Problem Formulation and Technical Analysis: Leaching is a liquid-solid separation process in which a solvent is used to extract the soluble constituents from a ground or crushed solid material. Such operations are

usually carried out in a countercurrent stagewise process since the single contacting of the two phases will result in a weak solution of the desired component and a low recovery. In countercurrent flows the solvent and solid are brought into contact, intimately mixed, and separated. The solvent phase, called the extract, becomes more concentrated as it passes through the stages toward the solid feed stage. The solid material and adhering solution, called the raffinate, moving towards the fresh solvent stage becomes successively less concentrated in soluble material. The solid material on a solute-free basis is referred to as the gangue.

The design of a leaching process involves the determination of the number of separation or mixing-settler stages which are required to effect the desired recovery of the valuable soluble solid constituents. The design equations, used to determine the number of separation stages, consist of the overall and component material balances for the entire process and then formulating the overall and component material balances for each separation stage. Also to be considered in the stagewise balances are any equilibrium conditions existing between the contacting streams. If the physical equilibrium conditions are not known, then experimentally determined relationships between the extract and raffinate must be known. Using Figure 1 as the example, the material balances are:

Total System:

Overall

$$F + S = R + E \tag{1}$$

Component

$$x_{iF}F + y_{iS}S = x_{iR}R + y_{iE}E \tag{2}$$

There exist C-1 component material balances, where C is the number of components, and one overall material balance. For each stream the sum of the mass or mole fractions must equal one. Similar balances exist around each stage where the output from one stage becomes the input to the next stage:

For the jth stage:

Overall Balance

$$R_{j-1} + F_{j+1} = R_j + E_j \tag{3}$$

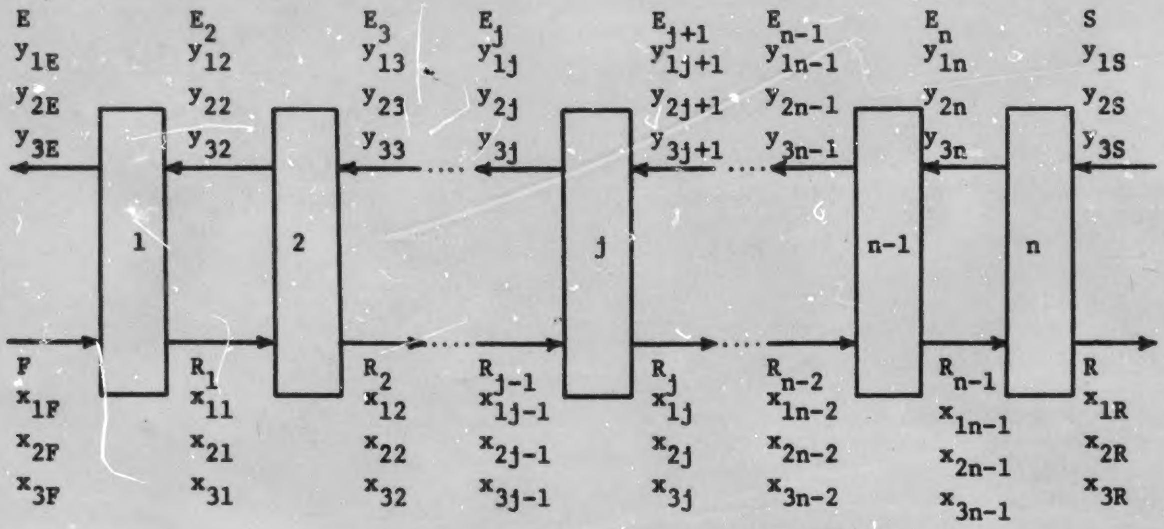
E
y_{1E}
y_{2E}
y_{3E}
E_2
y_{12}
y_{22}
y_{32}
E_3
y_{13}
y_{23}
y_{33}
E_j
y_{1j}
y_{2j}
y_{3j}
E_{j+1}
y_{1j+1}
y_{2j+1}
y_{3j+1}
E_{n-1}
y_{1n-1}
y_{2n-1}
y_{3n-1}
E_n
y_{1n}
y_{2n}
y_{3n}
S
y_{1S}
y_{2S}
y_{3S}
1
2
j
n-1
n
F
x_{1F}
x_{2F}
x_{3F}
R_1
x_{11}
x_{21}
x_{31}
R_2
x_{12}
x_{22}
x_{32}
R_{j-1}
x_{1j-1}
x_{2j-1}
x_{3j-1}
R_j
x_{1j}
x_{2j}
x_{3j}
R_{n-2}
x_{1n-2}
x_{2n-2}
x_{3n-2}
R_{n-1}
x_{1n-1}
x_{2n-1}
x_{3n-1}
R
x_{1R}
x_{2R}
x_{3R}

Figure 1. Schematic Flow Diagram of a Leaching Process

Component Balance

$$x_{ij-1} R_{j-1} + y_{ij+1} E_{j+1} = x_{ij} R_j + y_{ij} E_j \tag{4}$$

For the stagewise component balances R_j and E_j have a relation to each other, either equilibrium, or some experimentally established relation. For example, each pound of gangue in R_j might have 1.5 pounds of solution of composition y_j adhering to it. This must be considered when calculating the streams entering and leaving each stage.

For a three component system with two input and two output streams, three material balance equations and four mass fraction equations may be written about the entire process. There exist sixteen total material balance variables as shown in Figure 1 and listed in Table I. Thus for a unique solution to exist nine independent variables, or their equivalent must be specified. In the problem statement seven independent variables are specified as shown in Table I. For a unique solution two more independent variables must be determined. Indirectly these are given by (1) the specification of the fraction of solute recovered which allows E to be determined and (2) from the water to gangue ratio which along with (1) allows R to be determined. Thus a unique solution is available.

Table I. Total System Material Balance Variables in Leaching Process

		Composition		
Input Streams		Solute	Solvent	Gangue
Feed	F[*]	x_{1F}[*]	x_{2F}[*]	x_{3F}
Solvent	S	y_{1S}[*]	y_{2S}[*]	y_{3S}
Output Streams				
Extract	E	y_{1E}[*]	y_{2E}[*]	y_{3E}
Raffinate	R	x_{1R}	x_{2R}	x_{3R}

[*] Specified Variables

A similar analysis may be made about each stage. In this case the relation between R_j and E_j becomes the equivalent of a specified independent variable. The design of a leaching system requires that the number of equilibrium stages comprising the process be determined thus introducing another variable. This variable is found quite easily by adding stages until the solute recovery criteria are met.

A more difficult problem exists if the number of separation stages are specified. In this case one of the previously specified variables could not be a priori selected since the system would be over-specified. That is, the specified variables would not all be independent. Usually if the number of separation stages are specified, the solvent rate is determined by trial and error calculations until the material balance and solute recovery criteria are met. In this situation, for example, the composition of the extract product could not be specified. Doing so would result in an over-specified system. The problem statement may be reworded to ask what solvent rate is required and what is the solute mass fraction of the extract product stream if seven available separation stages are available. Note that in the stated problem where the number of separation stages are to be determined, the composition of the extract product stream is specified in order to have a unique solution.

3. Method of Solution: From the problem statement sufficient information is given to complete the overall and component balances about the entire system to determine the missing material stream values. The computer balances are calculated using the relation between the existing contacting streams and setting the input or output material streams from one stage equal to the output or input material streams respectively of the next stage calling stage one that in which the ore feed stream enters. For each set of stagewise calculations the amount of solute leaving in the raffinate stream, SOLFO, is compared to the solute leaving in the total system raffinate stream, SOLLO. When SOLFO is less than or equal SOLLO, the program terminates printing out the material stream quantities for each stage and indicating what number of stages are required.

In addition to the above calculations, if the number of available stages are specified, the program will adjust the value of the solvent rate by increments of 0.1 times the solvent rate until the number of calculated stages is equal to that specified. The program then uses the Newton method converging on SOLFO - SOLLO = 0 by iterating on the solvent rate. Newton's method requires the equation of interest to be written in implicit form and the first derivative of the equation be found. The approximate solution is found by:

1. Making a rough initial approximation of a value S_o of the solvent rate (S) which is close to the root of $f(S) = 0$. This is done by the computer for this leaching process program.
2. Use the equation

$$S_1 = S_o - \frac{f(S_o)}{f'(S_o)} \tag{5}$$

3. Use this technique consecutively to produce other approximations of the solution until two consecutive numbers agree to the desired accuracy. For example

$$S_2 = S_1 - \frac{f(S_1)}{f'(S_1)}, \ldots, S_{n+1} = S_n - \frac{f(S_n)}{f'(S_n)} \tag{6}$$

and $f(S_{n+1}) - f(S_n) = 0.01$, if this is the desired accuracy.

Newton's method for finding the roots of a function is not generally recommended unless the local structure of the function in the vicinity of the root is well understood and unless the first derivative can be found. To guarantee the success of this method, or convergence to the root, the following conditions are necessary:

1. An interval (a, b) within which the root is contained such that $f(a) \cdot f(b) < 0$. (opposite signs at ends of interval.)
2. $f'(S) \neq 0$, $a < S < b$. (monotonic within interval.)
3. $f''(S) \neq 0$, $a < S < b$. (no change of direction of concavity of curve within interval.)
4. $f(S_o) \cdot f''(S_o) > 0$. (the sign $f(S_o)$ must be the same as $f''(S_o)$ within the interval (S_o, S).)

In this problem the curve is well behaved and no convergence difficulties should arise even with a poorly selected first approximation of the solvent rate. Figure 2 shows the logic flow diagram for the computer solution.

4. References: The following references may be suggested to the students as sources of information:

1. Bennett, C.O., and J.E. Meyers, "Momentum, Heat and Mass Transfer," McGraw-Hill Book Company, New York, 1962.
2. Brown, G.G., et. al., "Unit Operations," John Wiley & Sons, New York, 1950.
3. Hamming, R.W., "Introduction to Applied Numerical Analysis," McGraw-Hill Book Company, 1971.
4. King, C.J., "Separation Processes," McGraw-Hill Book Company, New York, 1971.
5. McCabe, W.L., and J.C. Smith, "Unit Operations of Chemical Engineering," 2nd Ed., McGraw-Hill Book Company, New York, 1967.

5. Solution:

a. Results: The output format will depend upon the individual programmer since the students are asked to write the computer program. A typical output should resemble that of Figure 3 where the results are from the sample program included with this problem. Should the instructor so desire, the program as written may be used by the students rather than have the student do the programming.

NOTES:

NO - no. of specified stages by user
N - no. of calculated stages
diff - absolute value of calculated minus specified solute recovery
comp - absolute value of $S_{n+1} - S_n$
S_n - solvent feed rate calculated by Newton's method

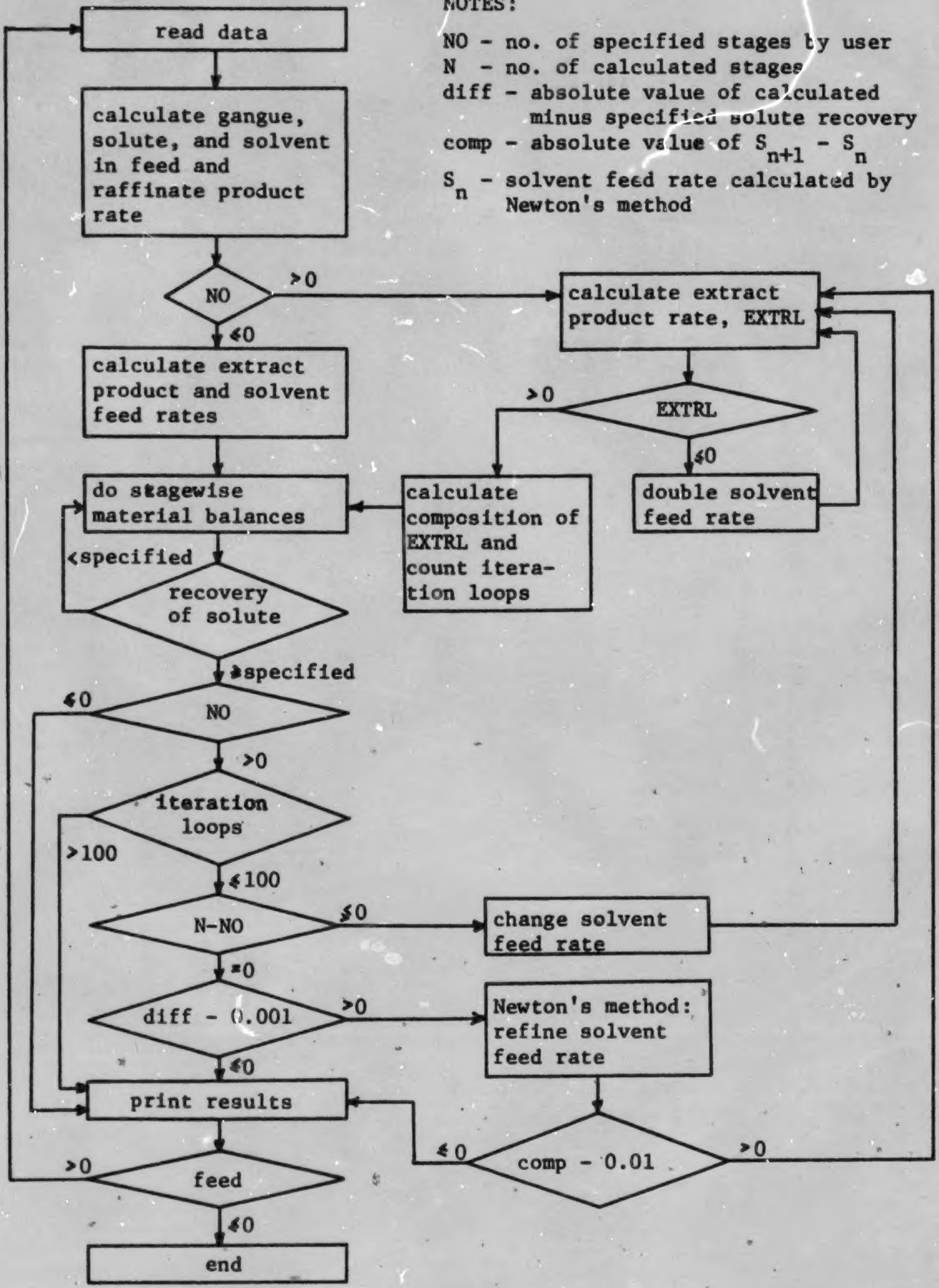
read data
calculate gangue, solute, and solvent in feed and raffinate product rate
NO
>0
≤0
calculate extract product and solvent feed rates
calculate extract product rate, EXTRL
EXTRL
>0
≤0
do stagewise material balances
calculate composition of EXTRL and count iteration loops
double solvent feed rate
<specified
recovery of solute
≥specified
≤0
NO
>0
iteration loops
>100
≤100
N-NO
≠0
change solvent feed rate
=0
diff - 0.001
>0
Newton's method: refine solvent feed rate
≤0
print results
≤0
comp - 0.01
>0
>0
feed
≤0
end

Figure 2. Computer Logic Diagram for LEACH

```
 INPUT DATA
100.00 100.00 0.0950 0.0500 0.8550 0.0000 1.0000 0.1000 0.9700  1.500          0


                    STAGEWISE CALCULATIONS FOR LEACHING PROCESS

                                 MATERIAL BALANCE

                         RAFFINATE                                  EXTRACT
STAGE        INPUT     FRAC       OUTPUT     FRAC         INPUT     FRAC        OUTPUT     FRAC
           TONS/DAY    CUSO4    TONS/DAY     CUSO4      TONS/DAY    CUSO4     TONS/DAY     CUSO4

  0         100.00    0.0950     214.03     0.0013       206.18    0.0000        92.14    0.1000

  1         100.00    0.0950     227.99     0.0625       220.14    0.0634        92.14    0.1000

  2         227.99    0.0625     222.43     0.0390       214.58    0.0391       220.14    0.0634

  3         222.43    0.0390     218.97     0.0238       211.12    0.0234       214.58    0.0391

  4         218.97    0.0238     216.82     0.0141       208.97    0.0133       211.12    0.0234

  5         216.82    0.0141     215.48     0.0080       207.63    0.0069       208.97    0.0133

  6         215.48    0.0080     214.65     0.0041       206.80    0.0029       207.63    0.0069

  7         214.65    0.0041     214.13     0.0017       206.28    0.0004       206.80    0.0029

  8         214.13    0.0017     213.81     0.0002       205.96   -0.0010       206.28    0.0004

 NOTE.. STAGE 0 REPRESENTS OVERALL MATERIAL BALANCE

  7  TO  8 THEORETICAL STAGES ARE REQUIRED
```

Figure 3. Solution and Output of Sample Problem by LEACH

b. Discussion of Results: This problem is intended as an exercise in material balance calculations using the concepts of stagewise processes. Equilibrium stages have been assumed although the program could be modified to account for the stagewise efficiencies. The results have physical consistency.

III. EDUCATIONAL (PEDOGOGICAL) ASPECTS

1. Description of Past Usage: Variations of this problem have been assigned to first semester junior students in a chemical engineering laboratory for the past three years. This laboratory is associated with a Heat-Mass Transfer lecture course. Students have been requested to write a general computer program to determine the number of stages required in a specific leaching process, an example of which is included in the Problem Statement.

2. Concepts Demonstrated: The intent of this problem is to (1) review material balances and simple equilibria, (2) introduce stagewise separation concepts and terminology, (3) demonstrate use of graphical techniques, (4) use simple numerical analysis techniques, and (5) reinforce the importance of a logical approach to the analysis and solution of engineering problems.

3. Evaluation of Usage: This has been a two week assignment, the second week overlapping a new experiment. It is my believe that this problem reemphasizes to the students the concept that material balances form the basis for many engineering calculations. In leaching processes the graphical solution technique, unless well understood, leads many students to looking for plug-in solutions rather than analyzing each problem. A tendency exists for students to use graphical techniques rather mechanically. The logic involved in writing the computer algorithm was found to be immensely educational since the operations had to be well thought out and careless or faulty thinking was pointedly brought to the students attention by poor computer results.

4. Nature of assignment: The problem was assigned to three man groups with the instructor available for consultation. Normally a short lecture on graphical techniques was also presented.

V. PROGRAM DESCRIPTION

1. General Description: The program consists of several subsections as shown in the logic flow diagram, Figure 2, and as outlined in Section II.3.

The program is limited, to using a feed rate less than 1,000 tons per day. Problems will be encountered if the number of stages are specified and the number of iteration loops are exceeded before convergence on the solvent rate is achieved. In this case a message is printed, "Number of iteration loops exceed 100, computations discontinued." The material balances, although unbalanced, are also printed. This difficulty can be overcome by changing the statement immediately following statement 61 to a larger number if so desired. The solvent rate must also be specified, preferably a two or three digit number since convergence has been difficult when 1.0 was used.

Further program description details are provided in the comment cards.

2. External Description: Details on the argument lists and data input format are provided on the comment cards.

3. Internal Description: a) Program variables -- a description is given on comment cards, b) Program logic -- the program logic is indicated by comment cards within the coding and is shown in Figure 2. c) Diagnostics -- no diagnostics are provided, except the indication that the number of iteration loops has exceeded that allowed before convergence occurs.

VI. PROGRAM LISTING

```
C     LEACH
C     MATERIAL BALANCES AND STAGEWISE CALCULATIONS FOR A LEACHING PROCESS
C     THIS PROGRAM CALCULATES THE OVERALL MATERIAL BALANCE AND STAGEWISE
C     MATERIAL BALANCES FOR A LEACHING PROCESS IN WHICH CUSO4 IS REMOVED FROM
C     ROASTED ORE.  THE RELATIOSHIP BETWEEN THE EXTRACT AND RAFFINATE STREAMS
C     IS SPECIFIED AS 'X' TONS OF WATER PER TON OF GANGUE.
C     TWO DIFFERENT CASES MAY BE SOLVED
C        1.  THE NUMBER OF EQUILIBRIUM STAGES REQUIRED TO EFFECT THE DESIRED
C            RECOVERY.
C        2.  GIVEN THE RECOVERY AND THE NUMBER OF SEPARATION STAGES AVAILABLE,
C            THE QUANTITY OF SOLVENT REQUIRED IS CALCULATED.
C     A SINGLE CARD OF INPUT INFORMATION HAVING THE FOLLOWING FORMAT IS REQUIRED
C           NAME                              VARIABLE     FORMAT        COLUMN
C     FRESH ROASTED ORE FEED                   FEED         F7.2           1-7
C     FRESH SOLVENT FEED                       SOLVT        F7.2          8-14
C     MASS FRAC. SOLUTE IN FEED                XSOLU        F7.4         15-21
C     MASS FRAC. SOLVENT IN FEED               XSOLV        F7.4         22-28
C     MASS FRAC. GANGUE IN FEED                XGANG        F7.4         29-35
C     MASS FRAC. SOLUTE IN FRESH SOLVENT       YSOLU        F7.4         36-42
C     MASS FRAC. SOLVENT IN FRESH SOLVENT      YSOLV        F7.4         43-49
C     MASS FRAC. SOLUTE IN PRODUCT EXTRACT     YEXTL        F7.4         50-56
C     FRACTION OF SOLUTE IN FEED RECOVERED     FRAC         F7.4         57-63
C     WEIGHT RATIO OF WATER TO GANGUE          RATIO        F7.3         64-70
C     NUMBER OF AVAILABLE STAGES               NO           I3           78-80
C     FOR CASE 1...THE NUMBER OF SEPARATION STAGES, NO, MUST BE ZERO.
C     FOR CASE 2...THE ESTIMATION OF THE SOLVENT RATE, SOLVT, AND THE NUMBER OF
C     AVAILABLE STAGES, NO, MUST BE SPECIFIED ON THE DATA INPUT CARD.
C     MORE THAN ONE PROBLEM MAY BE RUN PER PROGRAM DECK INPUT BY ADDING DATA
C     CARDS SEQUENTIALLY TO THE DATA DECK.  TO TERMINATE THE PROGRAM, THE FEED
C     MUST BE ZERO OR A BLANK CARD MUST BE USED AS THE LAST DATA CARD.
```

```
      DIMENSION FRRFI(20),FREXO(20),RAFFI(20),EXTRO(20),RAFFO(20)
      DIMENSION EXTRI(20),FRRFO(20),FREXI(20),DIFF(200)
      DATA IN,IOUT /5,6/
    1 READ(IN,110)FEED,SOLVT,XSOLU,XSOLV,XGANG,YSOLU,YSOLV,YEXTL,FRAC,
     1RATIO,NO
      WRITE(IOUT,118)FEED,SOLVT,XSOLU,XSOLV,XGANG,YSOLU,YSOLV,YEXTL,
     1FRAC,RATIO,NO
C     TOTAL MATERIAL BALANCE CALCULATIONS
      GANGE=XGANG*FEED
      SOLUT=XSOLU*FEED
      SOLV=XSOLV*FEED
      SOLUR=FRAC*SOLUT
      SOLLO=SOLUT-SOLUR
      RAFFS=GANGE*(1.+RATIO)
      RAFF=RAFFS+SOLLO
      XRAFF=SOLLO/RAFF
      K=0
      IF(NC) 20,20,501
  501 NC=NC+1
      GO TO 10
    9 SOLVT=2.*SOLVT
   10 EXTRL=FEED+SOLVT-RAFF
      IF(EXTRL) 9,9,12
   12 YEXTL=(SOLUR+YSOLU*SOLVT)/EXTRL
      K=K+1
      SNO=SOLVT
      GO TO 30
   20 EXTRL=SOLUR/YEXTL
      SOLVT=EXTRL+RAFF-FEED
   30 N=2
      FRRFI(N-1)=XSOLU
      FREXO(N)=YEXTL
      RAFFI(N-1)=FEED
      EXTRO(N)=EXTRL
C     END OF TOTAL MATERIAL BALANCE CALCULATIONS
```

```
C      STAGEWISE MATERIAL BALANCE CALCULATIONS
   40  SOLFO=(GANGE*RATIO/(1.-FREXO(N)))*FREXO(N)
       RAFFO(N)=RAFFS+SOLFO
       EXTRI(N+1)=RAFFO(N)+EXTRO(N)-RAFFI(N-1)
       FRRFO(N)=SOLFO/RAFFO(N)
       SOLFI=RAFFI(N-1)*FRRFI(N-1)
       SOLXO=EXTRO(N)*FREXO(N)
       SOLXI=SOLXO+SOLFO-SOLFI
       FREXI(N+1)=SOLXI/EXTRI(N+1)
       RAFFI(N)=RAFFO(N)
       FRRFI(N)=FRRFO(N)
       EXTRO(N+1)=EXTRI(N+1)
       FREXO(N+1)=FREXI(N+1)
       N=N+1
       IF(SOLFO-SOLLO) 50,50,40
C      END OF STAGEWISE MATERIAL BALANCE CALCULATIONS
   50  CONTINUE
       N=N-1
       IF(NC) 90,90,60
   60  CONTINUE
       IF(K-100) 61,61,69
   61  IF(N-NC) 70,62,80
C      NEWTON METHOD TO CONVERGE ON SPECIFIED SOLUTE RECOVERY BY ADJUSTING SOLVT
   62  DIFF(K)=SOLFO-SOLLO
       IF(ABS(DIFF(K))-0.001) 90,90,63
   63  FACT=SOLVT+FEED-RAFF-SOLUR
       SN1=SNO+(DIFF(K)*FACT**2.)/(GANGE*RATIO*SOLUR)
       SOLVT=SN1
       IF(ABS(SN1-SNO)-0.01) 90,90,10
C      END OF NEWTON METHOD
C      SOLVENT RATE ITERATIONS TO OBTAIN SPECIFIED NUMBER OF SEPARATION STAGES
   70  SOLVT=0.90*SOLVT
       GO TO 10
   80  SOLVT=1.10*SOLVT
       GO TO 10
   89 WRITE(IOUT,119)
   90 WRITE(IOUT,120)
      J=0
      WRITE(IOUT,130)J,FEED,XSOLU,RAFF,XRAFF,SOLVT,YSOLU,EXTRL,YEXTL
      DO 100 J=2,N
      L=J-1
      WRITE(IOUT,130)L,RAFFI(J-1),FRRFI(J-1),RAFFO(J),FRRFO(J),EXTRI(J+1
     1),FREXI(J+1),EXTRO(J),FREXO(J)
  100 CONTINUE
      WRITE(IOUT,140)
      N=N-1
      J=N-1
      IF(NC) 101,101,102
  101 WRITE(IOUT,150)J,N
      GO TO 159
  102 WRITE(IOUT,155)SOLVT,FEED
  110 FORMAT(2F7.2,7F7.4,F7.3,7X,I3)
  118 FORMAT(2X,10HINPUT DATA,/,2F7.2,7F7.4,F7.3,7X,I3,///)
  119 FORMAT(16X,66HNUMBER OF ITERATION LOOPS EXCEED 100. COMPUTATIONS D
     1ISCONTINUED....//)
  120 FORMAT(26X,43HSTAGEWISE CALCULATIONS FOR LEACHING PROCESS.//,38X,1
     16HMATERIAL BALANCE,//,25X,9HRAFFINATE,31X,7HEXTRACT,/,1X,5HSTAGE,2
     2(7X,5HINPUT,4X,4HFRAC,6X,6HOUTPUT,4X,4HFRAC ),/,7X,4(4X,8HTONS/DAY
     3,3X,5HCUSO4 ),/ )
  130 FORMAT(2XI3,2X4(4XF7.2,F9.4)/)
  140 FORMAT(2X,90HNOTE.. STAGE 0 REPRESENTS OVERALL MATERIAL BALANCE./)
  150 FORMAT(2XI3,2X,2HTO,I3,32H THEORETICAL STAGES ARE REQUIRED )
  155 FORMAT(2XF7.2,35H TONS/DAY OF WATER ARE REQUIRED PER,F7.2,17H TONS
     1/DAY OF FEED.///)
  159 IF(FEED)160,160,1
  160 CONTINUE
      WRITE(IOUT,170)
  170 FORMAT(2X20HEND OF CALCULATIONS.)
      STOP
      END
      DIMENSION FRRFI(20),FREXO(20),RAFFI(20),EXTRO(20),RAFFO(20)
      DIMENSION EXTRI(20),FRRFO(20),FREXI(20),DIFF(200)
      IN=2
      IOUT=3
    1 READ(IN,110)FEED,SOLVT,XSOLU,XSOLV,XGANG,YSOLU,YSOLV,YEXTL,FRAC,
     1RATIO,NO
      WRITE(IOUT,118)FEED,SOLVT,XSOLU,XSOLV,XGANG,YSOLU,YSOLV,YEXTL,
     1FRAC,RATIO,NO
C     TOTAL MATERIAL BALANCE CALCULATIONS
      GANGE=XGANG*FEED
      SOLUT=XSOLU*FEED
      SOLV=XSOLV*FEED
      SOLUR=FRAC*SOLUT
      SOLLO=SOLUT-SOLUR
      RAFFS=GANGE*(1.+RATIO)
      RAFF=RAFFS+SOLLO
      XRAFF=SOLLO/RAFF
      K=0
      IF(NO) 20,20,10
    9 SOLVT=2.*SOLVT
   10 EXTRL=FEED+SOLVT-RAFF
      IF(EXTRL) 9,9,12
   12 YEXTL=(SOLUR+YSOLU*SOLVT)/EXTRL
      K=K+1
      SNO=SOLVT
      GO TO 30
   20 EXTRL=SOLUR/YEXTL
      SOLVT=EXTRL+RAFF-FEED
   30 N=1
      FRRFI(N-1)=XSOLU
      FREXO(N)=YEXTL
      RAFFI(N-1)=FEED
      EXTRO(N)=EXTRL
C     END OF TOTAL MATERIAL BALANCE CALCULATIONS
```

```
C     STAGEWISE MATERIAL BALANCE CALCULATIONS
   40 SOLFO=(GANGE*RATIO/(1.-FREXO(N)))*FREXO(N)
      RAFFO(N)=RAFFS+SOLFO
      EXTRI(N+1)=RAFFO(N)+EXTRO(N)-RAFFI(N-1)
      FRRFO(N)=SOLFO/RAFFO(N)
      SOLFI=RAFFI(N-1)*FRRFI(N-1)
      SOLXO=EXTRO(N)*FREXO(N)
      SOLXI=SOLXO+SOLFO-SOLFI
      FREXI(N+1)=SOLXI/EXTRI(N+1)
      RAFFI(N)=RAFFO(N)
      FRRFI(N)=FRRFO(N)
      EXTRO(N+1)=EXTRI(N+1)
      FREXO(N+1)=FREXI(N+1)
      N=N+1
      IF(SOLFO-SOLLO) 50,50,40
C     END OF STAGEWISE MATERIAL BALANCE CALCULATIONS
   50 CONTINUE
      N=N-1
      IF(NO) 90,90,60
   60 CONTINUE
      IF(K-100) 61,61,89
   61 IF(N-NO) 70,62,80
C     NEWTON METHOD TO CONVERGE ON SPECIFIED SOLUTE RECOVERY BY ADJUSTING SOLVT
   62 DIFF(K)=SOLFO-SOLLO
      IF(ABS(DIFF(K))-0.001) 90,90,63
   63 FACT=SOLVT+FEED-RAFF-SOLUR
      SN1=SNO+(DIFF(K)*FACT**2.)/(GANGE*RATIO*SOLUR)
      SOLVT=SN1
      IF(ABS(SN1-SNO)-0.01) 90,90,10
C     END OF NEWTON METHOD
C     SOLVENT RATE ITERATIONS TO OBTAIN SPECIFIED NUMBER OF SEPARATION STAGES
   70 SOLVT=0.90*SOLVT
      GO TO 10
   80 SOLVT=1.10*SOLVT
      GO TO 10
   89 WRITE(IOUT,119)
   90 WRITE(IOUT,120)
      J=0
      WRITE(IOUT,130)J,FEED,XSOLU,RAFF,XRAFF,SOLVT,YSOLU,EXTRL,YEXTL
      DO 100 J=1,N
      WRITE(IOUT,130)J,RAFFI(J-1),FRRFI(J-1),RAFFO(J),FRRFO(J),EXTRI(J+1
     1),FREXI(J+1),EXTRO(J),FREXO(J)
  100 CONTINUE
      WRITE(IOUT,140)
      J=N-1
      IF(NO) 101,101,102
  101 WRITE(IOUT,150)J,N
      GO TO 159
  102 WRITE(IOUT,155)SOLVT,FEED
  110 FORMAT(2F7.2,7F7.4,F7.3,7X,I3)
  118 FORMAT(2X,10HINPUT DATA,/,2F7.2,7F7.4,F7.3,7X,I3,///)
  119 FORMAT(16X,66HNUMBER OF ITERATION LOOPS EXCEED 100, COMPUTATIONS D
     1ISCONTINUED...,///)
  120 FORMAT(26X,43HSTAGEWISE CALCULATIONS FOR LEACHING PROCESS,//,38X,1
     16HMATERIAL BALANCE,//,25X,9HRAFFINATE,31X,7HEXTRACT,/,1X,5HSTAGE,2
     22(7X,5HINPUT,4X,4HFRAC,6X,6HOUTPUT,4X,4HFRAC,),/,7X,4(4X,8HTONS/DAY
     3,3X,5HCUSO4,),/,)
  130 FORMAT(2XI3,2X4(4XF7.2,F9.4)/)
  140 FORMAT(2X,50HNOTE.. STAGE 0 REPRESENTS OVERALL MATERIAL BALANCE,/)
  150 FORMAT(2XI3,2X,2HTO,I3,32H THEORETICAL STAGES ARE REQUIRED,)
  155 FORMAT(2XF7.2,35H TONS/DAY OF WATER ARE REQUIRED PER,F7.2,17H TONS
     1/DAY OF FEED,///)
  159 IF(FEED)160,160,1
  160 CONTINUE
      WRITE(IOUT,170)
  170 FORMAT(2X20HEND OF CALCULATIONS.)
      CALL EXIT
      END
```

I. PROBLEM IDENTIFICATION

1. Title: Optimum Stages in Leaching
2. Author: Ning Hsing Chen
3. Affiliation: Lowell Technological Institute

II. TECHNICAL DESCRIPTION

1. Problem Statement: Determine the optimum number of theoretical stages and the optimum flow rate of solvent required for constant underflow leaching of a solid mixture to obtain the maximum profit of production.

2. Problem Formulation and Technical Analysis: The hourly profit of operating a cascade of leaching system under constant underflow to separate a valuable constituent from a solid mixture has been developed by the author (see reference) as

$$P_H = C_1 Sf\left[x_m - \frac{r-1}{r^m-1}(x_m - y_o) - y_o\right] - C_2 K'_F m(1+F) - tm - C_3 S - C_4 rSf \qquad (1)$$

in which

P_H	Hourly profit, \$/hr.
C_1	Unit cost of solute, \$/lb.
C_2	Unit cost of equipment, \$/stage
C_3	Unit cost of solid mixture, \$/lb.
C_4	Unit cost of solvent, \$/lb.
S	Flow rate of inert solid, lb./hr
f	Retention of liquid in sludge, lb. solution/lb. inert solid, or lb. solvent/lb. inert solid
w_o	Flow rate of fresh solvent to stage 1, lb./hr.
r	Ratio w_o/Sf
x_m	Composition of retention liquid in the sludge, lb. solute/lb. solution, or lb. solute/lb. solvent
y_o	Composition of solute in the overflow, lb. solute/lb. solution, or lb. solute/lb. solvent
m	Number of stages
F	Ratio of total cost to purchase cost of equipment

t	Hourly operating cost of one stage
K'_F	Ratio K_F/W
K_F	Fraction of initial cost
W	Hours of operation per year

3. Method of Solution: Differentiating Equation (1) with respect to m and r gives

$$\frac{\delta P_H}{\delta m} = C_1Sf\left[\frac{r-1}{(r^m-1)^2}\, r^m \ln r(x_m-y_o)\right]-C_2K'_F(1+F)-t \qquad (2)$$

$$\frac{\delta P_H}{\delta r} = C_1Sf(x_m-y_o)\left[\frac{(r-1)mr^{m-1}}{(r^m-1)^2} - \frac{1}{r^m-1}\right]- C_4 \qquad (3)$$

Equating Equations (2) and (3) to zero yields

$$G = r^{m+1}\ln r-r^m\ln r-P(r^m-1)^2 = 0 \qquad (4)$$

$$H = -Qr^{2m}+(m-1+2Q)r^m-mr^{m-1}+1-Q = 0 \qquad (5)$$

in which

$$P = \frac{C_2K'_F(1+F)+t}{(x_m-y_o)C_1Sf}$$

$$Q = \frac{C_4}{C_1(x_m-y_o)}$$

The derivatives of G and H in Equations (4) and (5) with respect to r and m, after simplification, are:

$$\frac{\delta G}{\delta r} = \left[(m+1)\ln r+1\right]r^m+(2mP-m\ln r-1)r^{m-1}-2mPr^{2m-1} \qquad (6)$$

$$\frac{\delta G}{\delta m} = r^{m+1}(\ln r)^2+\left[2P\ln r-(\ln r)^2\right]r^m-2Pr^{2m}\ln r \qquad (7)$$

$$\frac{\delta H}{\delta r} = (m^2-m+2mQ)r^{m-1}-m(m-1)r^{m-2}-2mQr^{2m-1} \qquad (8)$$

$$\frac{\delta H}{\delta m} = (m\ln r-\ln r+1+2Q\ln r)r^m-(m\ln r+1)r^{m-1}-2Qr^{2m}\ln r \qquad (9)$$

Then by the Newton Raphson method, the new values of m and r can be calculated by iteration as

$$r_{new} = r_{old} + \Delta r \qquad (10)$$

in which

$$r = \frac{G\frac{\delta H}{\delta m} - H\frac{\delta G}{\delta m}}{\frac{\delta H \delta G}{\delta r \delta m} - \frac{\delta H \delta G}{\delta m \delta r}}$$

and

$$m_{new} = m_{old} + \Delta m \qquad (11)$$

in which

$$m = \frac{H\frac{\delta G}{\delta r} - G\frac{\delta H}{\delta r}}{\frac{\delta H \delta G}{\delta r \delta m} - \frac{\delta H \delta G}{\delta m \delta r}}$$

The iteration is carried on until the absolute values of the Δr and Δm are smaller than a very small number. Then the optimum hourly profit is calculated from Equation (1).

4. References and Data: This problem with the same data appears on pages 71-74 of Chemical Engineering August 24, 1970 on "Optimum Theoretical Stages in Countercurrent Leaching" by Ning Hsing Chen

5. Solution:

a. Results: The computer output entitled "Optimum Stages in Leaching" contains the solutions of two examples. Both have the same input data as the one in the reference. The first one illustrates the failure of convergence with an estimate of the initial values of r=0.5 and m=5.00. The second shows that the identical results as the one in the reference are obtained with the initial values of r=0.96 and m=12.00.

b. Discussion of Results: Although convergence cannot always be obtained with any initial values, the iteration gives some hint on the next trial. To ensure the convergence, the initial values of r and m must meet the criteria of the Newton Raphson method.

III. EDUCATIONAL (PEDOGOLOGICAL) ASPECTS

1. Description of Past Udage: I have used this problem in my (senior level) plant design course for three years. The students have the option of using the graphical method as described in the reference.

2. Concepts Demonstrated: a0 Formulation of an economic objective function for computer solution, b) Application of the Newton Raphson method to solve nonlinear simultaneous equations.

3. Evaluation of Usage: This is a two week assignment. Student may change any pertinent data.

4. Nature of Assignment: The student is given a leaching problem. The instructor generally furnishes the initial values of r and m. This saves computer runs and the failure of convergence.

IV. PROGRAM SUMMARY SHEET

P

V. PROGRAM DESCRIPTION

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C     OPTIMUM STAGES IN LEACHING                                         MAIN  10
C     PROGRAMMED BY N.H.CHEN MARCH 9 1972 LOWELL TECHNOLOGICAL INSTITUTEMAIN  20
C*****                                                                  MAIN  30
C     MAIN PROGRAM                                                       MAIN  40
C*****                                                                  MAIN  50
C     PURPOSE                                                            MAIN  60
C*****                                                                  MAIN  70
C     DRIVER PROGRAM. READS IN COST DATA,FLOW RATE OF INERT,RETENTION OFMAIN  80
C     LIQUID,COMPOSITION OF RETENTION LIQUID,AND OF SOLUTE AND OTHERS   MAIN  90
C     AND SOLVE FOR THE OPTIMUM STAGES AND SO FORTH AND OUTPUTS THE     MAIN 100
C     RESULTS.                                                          MAIN 110
C*****                                                                  MAIN 120
C     DESCRIPTION OF IMPORTANT VARIABLES                                MAIN 130
C*****                                                                  MAIN 140
C     AKF       FRACTION OF INITIAL COST                                MAIN 150
C     AKPRI     RATIO AKF TO W                                          MAIN 160
C     ALPHA     VARIABLE CONTROLLING RATIO AND NUMBER OF STAGES         MAIN 170
C     AM        NUMBER OF STAGES                                        MAIN 180
C     C1        UNIT COST OF SOLUTE,$/LB.                               MAIN 190
C     C2        UNIT COST OF EQUIPMENT,$/STAGE                          MAIN 200
C     C3        UNIT COST OF SOLID MIXTURE,$/LB.                        MAIN 210
C     C4        UNIT COST OF SOLVENT,$/LB.                              MAIN 220
C     F         RATIO OF TOTAL COST TO PURCHASE COST OF EQUIPMENT       MAIN 230
C     KAPPA     VARIABLE CONTROLLING NUMBER OF ITERATIONS               MAIN 240
C     PH        HOURLY PROFIT,$/HR.                                     MAIN 250
C     R         RATIO WO/S/SMF                                          MAIN 260
C     S         FLOW RATE OF INERT SOLID,LB./HR.                        MAIN 270
C     SMF       RETENTION OF LIQUID IN SLUDGE,LB. SOLUTION/LB. INERT    MAIN 280
C               SOLID,OR LB. SOLVENT/LB. INERT SOLID                    MAIN 290
C     T         HOURLY OPERATING COST OF ONE STAGE,$/HR.                MAIN 300
C     W         HOURS OF OPERATION PER YEAR,HR./YR.                     MAIN 310
C     WO        FLOW RATE OF FRESH SOLVENT TO STAGE 1,LB./HR.           MAIN 320
C     XM        COMPOSITION OF RETENTION LIQUID IN THE SLUDGE AT STAGE M MAIN 330
C     YO        COMPOSITION OF SOLUTE IN THE OVERFLOW                   MAIN 340
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C*****                                                                  MAIN 350
C     DATA INPUT                                                        MAIN 360
C*****                                                                  MAIN 370
C                        VARIABLES                     FORMAT           MAIN 380
C                                                                       MAIN 390
C     1.  FIRST CARD     C1,S,SMF,XM,YO,C2,AKPRI     6F10.4,F10.5       MAIN 400
C                                                                       MAIN 410
C     2.  SECOND CARD    F,T,C3,C4,W,ALPHA           6F10.4,F10.5       MAIN 420
C                                                                       MAIN 430
C     3.  THIRD CARD     R,AM,KAPPA                  F10.2,F5.2,I3      MAIN 440
C*****                                                                  MAIN 450
C     OUTPUT                                                            MAIN 460
C*****                                                                  MAIN 470
C     1.  OPTIMUM RATIO R                                               MAIN 480
C                                                                       MAIN 490
C     2.  OPTIMUM STAGES,AM                                             MAIN 500
C                                                                       MAIN 510
C     3.  HOURLY PROFIT,PH                                              MAIN 520
C                                                                       MAIN 530
C     4.  OPTIMUM SOLVENT RATE,WO                                       MAIN 540
C*****                                                                  MAIN 550
C     LIMITATIONS                                                       MAIN 560
C*****                                                                  MAIN 570
C     1.  CONSTANT UNDERFLOW LEACHING                                   MAIN 580
C                                                                       MAIN 590
C     2.  INITIAL VALUES OF R AND AM MUST MEET THE CRITERIA OF NEWTON   MAIN 600
C                                                                       MAIN 610
C         RAPHSON METHOD OF SOLVING NONLINEAR SYSTEM OF EQUATIONS       MAIN 620
C*****                                                                  MAIN 630
      WRITE(5,1)                                                        MAIN 640
    1 FORMAT(10X,26HOPTIMUM STAGES IN LEACHING)                         MAIN 650
      READ(6,2)C1,S,SMF,XM,YO,C2,AKPRI                                  MAIN 660
      READ(6,2)F,T,C3,C4,W,ALPHA                                        MAIN 670
    2 FORMAT(6F10.4,F10.5)                                              MAIN 680
      WRITE(5,22)                                                       MAIN 690
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   22 FORMAT(3X,10HINPUT DATA)                                          MAIN 700
      WRITE(5,5)                                                        MAIN 710
    5 FORMAT(4X,2HC1,9X,1HS,7X,3HSMF,8X,2HXM,8X,2HYO,8X,2HC2,7X,5HAKPRI)MAIN 720
      WRITE(5,9)C1,S,SMF,XM,YO,C2,AKPRI                                 MAIN 730
    9 FORMAT(7E10.2)                                                    MAIN 740
      WRITE(5,6)                                                        MAIN 750
    6 FORMAT(6X,1HF,11X,1HT,7X,2HC3,10X,2HC4,11X,1HW,10X,5HALPHA)       MAIN 760
      WRITE(5,8)F,T,C3,C4,W,ALPHA                                       MAIN 770
    8 FORMAT(6E12.4/)                                                   MAIN 780
  999 NR=0                                                              MAIN 790
      READ(6,3)R,AM,KAPPA                                               MAIN 800
    3 FORMAT(F10.2,F5.2,I3)                                             MAIN 810
      WRITE(5,7)R,AM,KAPPA                                              MAIN 820
    7 FORMAT(10X,3HR= ,F10.2,10X,4HAM= ,F9.2,10X,7HKAPPA= ,I3//)        MAIN 830
      WRITE(5,333)                                                      MAIN 840
  333 FORMAT(3X,14HOUTPUT RESULTS)                                      MAIN 850
   88 X=R                                                               MAIN 860
      Y=AM                                                              MAIN 870
      A=X**Y                                                            MAIN 880
      B=ALOG(X)                                                         MAIN 890
      P=(C2*AKPRI*(1.+F)+T)/((XM-YO)*C1*S*SMF)                          MAIN 900
      Q=C4/(C1*(XM-YO))                                                 MAIN 910
      H=-Q*A**2.+(Y-1.+2.*Q)*A-Y*A/X+1.-Q                               MAIN 920
      DHR=(Y**2.-Y+2.*Y*Q)*A/X-Y*(Y-1.)*A/X**2.-2.*Y*Q*A**2./X          MAIN 930
      DHM=(Y*B-B+1.+2.*Q*B)*A-(Y*B+1.)*A/X-2.*Q*B*A**2.                 MAIN 940
      G=A*X*B-A*B-P*(A-1.)**2                                           MAIN 950
      DGR=((Y+1.)*B+1.)*A+(2.*Y*P-Y*B-1.)*A/X-2.*Y*P*A**2./X            MAIN 960
      DGM=A*X*B*B+(2.*P*B-B*B)*A-2.*P*B*A*A                             MAIN 970
      WRITE(5,33)                                                       MAIN 980
   33 FORMAT(8X,1HH,8X,1HG,8X,3HDHR,8X,3HDHM,8X,3HDGR,8X,3HDGM,4X,2HNR) MAIN 990
      WRITE(5,44)H,G,DHR,DHM,DGR,DGM,NR                                 MAIN1000
   44 FORMAT(2X,6E10.4,I6)                                              MAIN1010
      D=DHR*DGM-DHM*DGR                                                 MAIN1020
      ALFAX=(G*DHM-H*DGM)/D                                             MAIN1030
      ALFAY=(H*DGR-G*DHR)/D                                             MAIN1040
      NR=NR+1                                                           MAIN1050
      R=X+ALFAX                                                         MAIN1060
      AM=Y+ALFAY                                                        MAIN1070
      WRITE(5,55)                                                       MAIN1080
   55 FORMAT(8X,1HD,8X,5HALFAX,8X,5HALFAY,8X,2H R,8X,2HAM)                 MAIN1090
      WRITE(5,66) D,ALFAX,ALFAY,R,AM                                    MAIN1100
   66 FORMAT(3X,5E12.4)                                                 MAIN1110
      IF(NR-KAPPA) 65,65,98                                             MAIN1120
   65 IF(ABS(ALFAY)-ALPHA) 12,12,88                                     MAIN1130
   12 IF(ABS(ALFAX)-ALPHA) 11,11,88                                     MAIN1140
   11 PH=C1*S*SMF*(XM-(R-1.)*(XM-YO)/(R**AM-1.)-YO)-C2*AKPRI*AM*(1.+F)- MAIN1150
     1T*AM-C3*S-C4*R*S*SMF                                              MAIN1160
      WO=R*S*SMF                                                        MAIN1170
      WRITE(5,4)                                                        MAIN1180
    4 FORMAT(8X,1HR,14X,2HAM,13X,2HPH,13X,2HWO)                         MAIN1190
      WRITE(5,56) R,AM,PH,WO                                            MAIN1200
   56 FORMAT(4E15.4)                                                    MAIN1210
      GO TO 10                                                          MAIN1220
   98 WRITE(5,300)                                                      MAIN1230
  300 FORMAT(10X,39HFAILED TO CONVERGE AFTER 25 ITERATIONS.///)         MAIN1240
      GO TO 999                                                         MAIN1250
   10 STOP                                                              MAIN1260
```

```
        OPTIMUM STAGES IN LEACHING
  INPUT DATA
   C1           S          SMF          XM          YO          C2        AKPRI
 0.15E+01  0.40E+04  0.20E+01  0.56E-01  0.00E+00  0.50E+05  0.30E-04
    F              T          C3            C4              W           ALPHA
 0.1500E+01  0.2500E+00  0.5000E-02  0.4000E-01  0.8400E+04  0.1000E-02

          R=        0.50            AM=        5.00            KAPPA=  25


  OUTPUT RESULTS
        H            G             DHR            DHM            DGR             DGM      NR
  0.312E+00 0.457E-02-0.927E+00 0.763E-01 0.594E-01-0.779E-02         0
        D           ALFAX            ALFAY             R             AM
    0.2683E-02  0.1036E+01  0.8492E+01  0.1536E+01  0.1349E+02
        H            G             DHR            DHM            DGR             DGM      NR
 -0.553E+05-0.631E+03-0.983E+06-0.480E+05-0.115E+05-0.575E+03         1
        D           ALFAX            ALFAY             R             AM
    0.1244E+08 -0.1230E+00  0.1369E+01  0.1413E+01  0.1486E+02
        H            G             DHR            DHM            DGR             DGM      NR
 -0.146E+05-0.166E+03-0.314E+06-0.103E+05-0.365E+04-0.124E+03         2
        D           ALFAX            ALFAY             R             AM
    0.1147E+07 -0.8632E-01  0.1212E+01  0.1326E+01  0.1687E+02
        H            G             DHR            DHM            DGR             DGM      NR
 -0.430E+04-0.486E+02-0.108E+06-0.251E+04-0.125E+04-0.303E+02         3
        D           ALFAX            ALFAY             R             AM
    0.1283E+06 -0.6172E-01  0.9397E+00  0.1265E+01  0.1701E+02
        H            G             DHR            DHM            DGR             DGM      NR
 -0.138E+04-0.156E+02-0.391E+05-0.681E+03-0.450E+03-0.827E+01         4
        D           ALFAX            ALFAY             R             AM
    0.1703E+05 -0.4538E-01  0.5854E+00  0.1219E+01  0.1760E+02
```

```
      H              G             DHR            DHM            DGR            DGM      NR
-0.466E+03-0.531E+01-0.146E+05-0.200E+03-0.167E+03-0.247E+01                              5
      D          ALFAX           ALFAY          R           AM
   0.2576E+04 -0.3476E-01  0.2097E+00  0.1184E+01  0.1781E+02
      H              G             DHR            DHM            DGR            DGM      NR
-0.153E+03-0.167E+01-0.554E+04-0.621E+02-0.531E+02-0.785E+00                              6
      D          ALFAX           ALFAY          R           AM
   0.4301E+03 -0.2810E-01 -0.1251E+00  0.1156E+01  0.1768E+02
      H              G             DHR            DHM            DGR            DGM      NR
-0.584E+02-0.673E+00-0.212E+04-0.200E+02-0.239E+02-0.262E+00                              7
      D          ALFAX           ALFAY          R           AM
   0.7576E+02 -0.2300E-01 -0.3784E+00  0.1132E+01  0.1730E+02
      H              G             DHR            DHM            DGR            DGM      NR
-0.214E+02-0.243E+00-0.815E+03-0.657E+01-0.908E+01-0.908E-01                              8
      D          ALFAX           ALFAY          R           AM
   0.1431E+02 -0.2144E-01 -0.5379E+00  0.1111E+01  0.1677E+02
      H              G             DHR            DHM            DGR            DGM      NR
-0.754E+01-0.879E-01-0.316E+03-0.217E+01-0.346E+01-0.325E-01                              9
      D          ALFAX           ALFAY          R           AM
   0.2742E+01 -0.1967E-01 -0.6119E+00  0.1091E+01  0.1615E+02
      H              G             DHR            DHM            DGR            DGM      NR
-0.269E+01-0.314E-01-0.124E+03-0.716E+00-0.133E+01-0.120E-01                             10
      D          ALFAX           ALFAY          R           AM
   0.5325E+00 -0.1813E-01 -0.6182E+00  0.1073E+01  0.1554E+02
      H              G             DHR            DHM            DGR            DGM      NR
-0.946E+00-0.111E-01-0.463E+02-0.233E+00-0.514E+00-0.453E-02                             11
      D          ALFAX           ALFAY          R           AM
   0.1037E+00 -0.1646E-01 -0.5755E+00  0.1057E+01  0.1496E+02
      H              G             DHR            DHM            DGR            DGM      NR
-0.327E+00-0.382E-02-0.200E+02-0.745E-01-0.293E+00-0.176E-02                             12
      D          ALFAX           ALFAY          R           AM

   0.2003E-01 -0.1448E-01 -0.5020E+00  0.1042E+01  0.1446E+02
```

```
        H           G           DHR           DHM           DGR           DGM       NR
-0.110E+00-0.129E-02-0.827E+01-0.231E-01-0.824E-01-0.689E-03                        13
        D          ALFAX            ALFAY            R           AM
     0.3794E-02 -0.1221E-01 -0.4130E+00  0.1030E+01  0.1405E+02
        H           G           DHR           DHM           DGR           DGM       NR
-0.363E-01-0.423E-03-0.349E+01-0.693E-02-0.346E-01-0.268E-03                        14
        D          ALFAX            ALFAY            R           AM
     0.6967E-03 -0.9755E-02 -0.3211E+00  0.1020E+01  0.1372E+02
        H           G           DHR           DHM           DGR           DGM       NR
-0.116E-01-0.134E-03-0.151E+01-0.199E-02-0.151E-01-0.101E-03                        15
        D          ALFAX            ALFAY            R           AM
     0.1225E-03 -0.7333E-02 -0.2353E+00  0.1013E+01  0.1349E+02
        H           G           DHR           DHM           DGR           DGM       NR
-0.354E-02-0.412E-04-0.672E+00-0.551E-03-0.687E-02-0.360E-04                        16
        D          ALFAX            ALFAY            R           AM
     0.2040E-04 -0.5144E-02 -0.1618E+00  0.1008E+01  0.1333E+02
        H           G           DHR           DHM           DGR           DGM       NR
-0.104E-02-0.121E-04-0.307E+00-0.147E-03-0.324E-02-0.120E-04                        17
        D          ALFAX            ALFAY            R           AM
     0.3194E-05 -0.3351E-02 -0.1034E+00  0.1004E+01  0.1322E+02
        H           G           DHR           DHM           DGR           DGM       NR
-0.293E-03-0.340E-05-0.144E+00-0.380E-04-0.157E-02-0.368E-05                        18
        D          ALFAX            ALFAY            R           AM
     0.4690E-06 -0.2023E-02 -0.6227E-01  0.1002E+01  0.1316E+02
        H           G           DHR           DHM           DGR           DGM       NR
-0.801E-04-0.921E-06-0.691E-01-0.970E-05-0.772E-03-0.105E-05                        19
        D          ALFAX            ALFAY            R           AM
     0.6520E-07 -0.1157E-02 -0.2579E-01  0.1001E+01  0.1314E+02
        H           G           DHR           DHM           DGR           DGM       NR
-0.212E-04-0.239E-06-0.334E-01-0.244E-05-0.384E-03-0.280E-06                        20
        D          ALFAX            ALFAY            R           AM
     0.8414E-08 -0.6377E-03  0.1950E-01  0.1001E+01  0.1316E+02
```

```
      H          G           DHR          DHM          DGR          DGM      NR
-0.574E-05-0.588E-07-0.158E-01-0.579E-06-0.191E-03-0.671E-07      21
      D          ALFAX          ALFAY          R          AM
   0.9500E-09 -0.3199E-03  0.3578E-01  0.1000E+01  0.1319E+02
      H          G           DHR          DHM          DGR          DGM      NR
-0.122E-05-0.141E-07-0.747E-02-0.119E-06-0.953E-04-0.155E-07      22
      D          ALFAX          ALFAY          R          AM
   0.1348E-10 -0.1652E-03  0.1059E+00  0.1000E+01  0.1330E+02
      H          G           DHR          DHM          DGR          DGM      NR
-0.122E-05-0.378E-08-0.331E-02-0.339E-07-0.471E-04-0.306E-08      23
      D          ALFAX          ALFAY          R          AM
   0.8522E-11 -0.4259E-03  0.5550E+01  0.9997E+00  0.1885E+02
      H          G           DHR          DHM          DGR          DGM      NR
-0.194E-05-0.118E-06 0.121E-01-0.147E-05 0.801E-03-0.217E-07      24
      D          ALFAX          ALFAY          R          AM
  -0.1456E-09  0.1649E-03  0.7795E+00  0.9999E+00  0.1963E+02
      H          G           DHR          DHM          DGR          DGM      NR
-0.298E-07-0.248E-07 0.558E-02 0.118E-07 0.394E-03-0.414E-08      25
      D          ALFAX          ALFAY          R          AM
  -0.2773E-10  0.1498E-04 -0.4572E+01  0.9999E+00  0.1505E+02
          FAILED TO CONVERGE AFTER 25 ITERATIONS.
```

```
       R=        0.96             AM=     12.00            KAPPA=  25

OUTPUT RESULTS
     H          G            DHR          DHM          DGR          DGM     NR
0.938E-03 0.524E-06-0.346E+00 0.166E-02 0.151E-02-0.170E-03       0


     D          ALFAX          ALFAY          R           AM
  0.5637E-04  0.2845E-02  0.2842E-01  0.9628E+00  0.1203E+02
     H          G            DHR          DHM          DGR          DGM     NR
0.899E-04-0.308E-07-0.280E+00 0.132E-02 0.130E-02-0.151E-03       1
     D          ALFAX          ALFAY          R           AM
  0.4055E-04  0.3334E-03  0.2678E-02  0.9632E+00  0.1203E+02
     H          G            DHR          DHM          DGR          DGM     NR
0.116E-05-0.960E-09-0.272E+00 0.128E-02 0.128E-02-0.149E-03       2
     D          ALFAX          ALFAY          R           AM
  0.3888E-04  0.4414E-05  0.3147E-04  0.9632E+00  0.1203E+02
     R              AM               PH               WO
  0.9632E+00      0.1203E+02      0.1628E+03      0.7705E+04
```

I. PROBLEM IDENTIFICATION

1. Title: Countercurrent Multi-Stage Solid-Liquid Extraction
2. Author: Charles M. Thatcher
3. Affiliation: University of Arkansas

II. TECHNICAL DESCRIPTION

1. Problem Statement: Vegetable oil is to be recovered from 4,000 pounds per hour of a vegetable mash by countercurrent extraction with 7,000 pounds per hour of a solvent. The mash analyzes 55 per cent oil, and it is estimated that the fresh solvent fed to the process will contain 4 per cent oil. The underflow stream leaving the bottom of each stage will retain 0.9 pounds of solution per pound of oil-free mash.

Calculate the component and total-mass quantities for all streams in a single-stage, a two-stage, and a three-stage process. Also calculate and compare the extract solute concentration and the percentage of total input oil which is lost to the raffinate product in each case.

2. Problem Formulation and Technical Analysis: This is a typical multi-stage mass balance problem in which component quantities must be specified or calculated for each of 2N + 2 process streams, where N is the number of stages in the process. For the present case of three components--solvent, oil, and insoluble mash--there would appear to be 6N + 6 quantities of interest. Of these, six are specified in the problem statement, leaving 6N to be determined.

The problem is first simplified by recognizing that the mass balance analysis for the insoluble mash is trivial: The N extract streams are all assumed to be free of insoluble mash, and each raffinate stream must therefore contain a quantity of insoluble mash equal to that present in the feed, which is known. This analysis reduces the number of remaining unknown quantities to 4N: the quantity of solvent and of oil in each of N extract and N raffinate streams.

The N stages correspond to N independent mass-balance systems and, for the reduced case of a two-component process, there are two independent mass balances applicable to each such system. Thus a total of 2N mass balance equations must be satisfied, leaving 2N additional relationships to be identified to permit the calculation of the 4N unknown quantities.

An application of the given solution-to-insolubles ratio to each underflow stream coupled with the imposition of the "equilibrium" requirement to each stage provides the needed 2N additional relationships. The equilibrium requirement in this case is that the extract solution leaving each stage have the same composition as the raffinate solution leaving that same stage.

Because the equilibrium requirement involves composition, it will be advantageous to introduce the oil mass fraction in each stream into the calculations. If the total mass of each liquid stream is also introduced, a change in primary unknown quantities can be effected: The quantity of oil and of solvent--the original unknowns--in any liquid stream is readily calculable once the total mass and oil mass fraction have been determined for that stream. With this change, then, the 4N unknown quantities become the total mass and oil mass fraction in each of 2N liquid streams.

The foregoing change of primary unknowns permits the direct imposition of the equilibrium requirement that the extract and raffinate streams leaving any given stage have identical oil mass fractions. The result is an effective reduction in total unknown quantities from 4N to 3N: 2N total mass quantities, and N oil mass fractions. The corresponding equations are 2N mass balance relationships and N applications of the given solution-to-insolubles ratio.

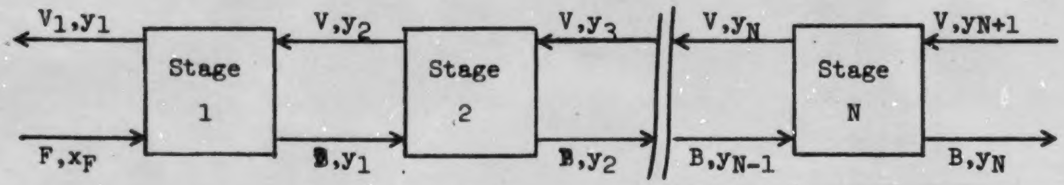
3. Method of Solution: As is suggested by the foregoing analysis, the first step in the solution is to complete the insolubles balance to obtain the quantity of insoluble mash in each raffinate stream. With no insoluble material in any of the extract streams, the insoluble mash in the feed is carried from each raffinate stream to the next, making the insoluble quantity the same for all such streams. The quantity will be equal to $F(1 - x_F)$, where F is the feed quantity and x_F the oil mass fraction in the feed.

The given solution-to-insolubles ratio, to be denoted by R, may then be applied to determine the quantity of solution in each raffinate stream: $R \cdot F(1 - x_F)$. The quantity of solution in each extract stream is then obtainable from successive total-mass balances written around each stage, starting at the raffinate product end of the process. It will be found that, with the sole exception of the final extract product, all extract quantities--including the solvent feed--are the same. Let these identical quantities be denoted by V, and the extract product quantity by V_1.

With all total-mass quantities known, only the N oil mass fractions remain to be calculated. Oil balances around each of the N stages provide the N relationships to be solved simultaneously for the N unknown mass fractions. Any suitable technique, including trial-and-error, might be used to solve this set of equations.

Whatever method of solution is selected, the calculations can be simplified by a redefinition of the N independent systems around which oil balances are to be written: Let the first balance be written around the first stage, the second around the first two stages, the third around the first three stages, etc., with the Nth balance to be written around all N stages--i.e., an overall mass balance.

This modification makes it possible to derive a generalized solution as follows:



Known quantities: feed quantity F and oil mass fraction x_F, solvent feed and extract quantities V, oil mass fraction in solvent feed y_{N+1}, extract product quantity V_1, raffinate solution-to-insolubles ratio R, raffinate liquid quantities $B = R\cdot F(1 - x_F)$.

Oil balance, 1st stage: $Fx_F + Vy_2 = V_1y_1 + By_1$

or, $$y_2 = \frac{B}{V}y_1 + \left(\frac{V_1y_1 - Fx_F}{V}\right) = Ay_1 + C \quad \text{(defines A and C)} \qquad (1)$$

Oil balance, stages 1-2: $Fx_F + Vy_3 = V_1y_1 + By_2$

$$y_3 = \frac{B}{V}y_2 + \left(\frac{V_1y_1 - Fx_F}{V}\right) = Ay_2 + C, \quad \text{from above definitions}$$

Using Eq. (1) to eliminate y_2, $$y_3 = A^2y_1 + (1 + A)C \qquad (2)$$

Similarly, for stages 1-3,

$$y_4 = Ay_3 + C = A^3y_1 + (1 + A + A^2)C \qquad (3)$$

From the pattern established by Eqs. (1) through (3), it can be seen that a balance around the first i stages will yield

$$y_{i+1} = A^i y_1 + (1 + A + A^2 + \ldots + A^{i-1})C$$
$$= A^i y_1 + S_{i-1}C \qquad \text{(defines S)} \qquad (4)$$

and, for N stages,

$$y_{N+1} = A^N y_1 + S_{N-1}C$$
$$= A^N y_1 + S_{N-1}\left(\frac{V_1 y_1 - Fx_F}{V}\right) \qquad (5)$$

from the definition of C. Eq. (5) can be solved for y_1 to obtain

$$y_1 = \frac{Vy_{N+1} + S_{N-1}Fx_F}{VA^N + S_{N-1}V_1} \qquad (6)$$

The foregoing derivation provides the basis for a complete numerical solution to the problem:

1) Evaluate $A = B/V$ and the successive powers of A up through A^N.
2) Evaluate the successive partial sums, S_1 through S_{N-1}, of the series $1 + A + A^2 + \ldots + A^{N-1}$.
3) Substitute known and calculated values into Eq. (6) and calculate the value of y_1.
4) Calculate the value of C, as defined in Eq. (1).
5) Successively calculate the values of y_2 through y_N by means of Eq. (4), using the appropriate values of A^i and S_{i-1} obtained in steps (1) and (2) above.

(This method of solution is directly analogous to the absorption factor method applicable to vapor-liquid equilibrium calculations as applied to absorption and stripping operations.)

4. References and Data: This problem is based on Problems 13-2 and 13-3, page 341, of "Fundamentals of Chemical Engineering", by C. M. Thatcher. For additional information on the absorption-factor method, see pp111-112 of "Mass Transfer Operations", second edition, by R. E. Treybal.

5. Solution:

a. Results: The calculated results for the three cases specified--that is, for single-stage, two-stage, and three-stage processes --are presented in the accompanying tables. The column and line headings make the presentation self-explanatory.

```
ECHO PRINT OF INPUT DATA:

4000.     .55       7000.     .04       .9
 1
 2
 3
 0
```

```
PRINTED OUTPUT FOR 1, 2, AND 3 STAGES:

                        MASS BALANCE, MULTI-STAGE EXTRACTION

GIVEN    FEED =  4000. LBS/HR, 0.550 LBS SOLUTE PER LB FEED
         SOLVENT FEED =  7000. LBS/HR, 0.040 LBS SOLUTE PER LB SOLVENT FEED
         0.90 LBS LIQUID PER LB SOLID IN UNDERFLOW

         BASIS 1 HOUR        V IN        L IN*        V OUT       L OUT*

         STAGE  1 OF  1
           TOTAL LBS        7000.0      2200.0       7580.0      1620.0
           LBS SOLVENT      6720.0         0.0       5536.7      1183.3
           LBS SOLUTE        280.0      2200.0       2043.3       436.7
           SOLUTE FRAC.      0.040       1.000        0.270       0.270

              * ALL L STREAMS ALSO CONTAIN  1800.0 LBS SOLID

           UNRECOVERED FRACTION OF TOTAL SOLUTE ENTERING = 0.177
```

```
                 MASS BALANCE, MULTI-STAGE EXTRACTION

GIVEN   FEED =  4000. LBS/HR, 0.550 LBS SOLUTE PER LB FEED
        SOLVENT FEED =  7000. LBS/HR, 0.040 LBS SOLUTE PER LB SOLVENT FEED
        0.90 LBS LIQUID PER LB SOLID IN UNDERFLOW

        BASIS 1 HOUR        V IN       L IN*       V OUT       L OUT*

        STAGE  1 OF  2
          TOTAL LBS       7000.0      2200.0      7580.0      1620.0
          LBS SOLVENT     6367.6         0.0      5246.3      1121.3
          LBS SOLUTE       632.4      2200.0      2333.6       498.7
          SOLUTE FRAC.     0.090       1.000       0.308       0.308

        STAGE  2 OF  2
          TOTAL LBS       7000.0      1620.0      7000.0      1620.0
          LBS SOLVENT     6720.0      1121.3      6367.6      1473.6
          LBS SOLUTE       280.0       498.7       632.4       146.4
          SOLUTE FRAC.     0.040       0.308       0.090       0.090

           * ALL L STREAMS ALSO CONTAIN  1800.0 LBS SOLID

          UNRECOVERED FRACTION OF TOTAL SOLUTE ENTERING = 0.060
```

```
                    MASS BALANCE, MULTI-STAGE EXTRACTION

GIVEN   FEED =  4000. LBS/HR, 0.550 LBS SOLUTE PER LB FEED
        SOLVENT FEED =  7000. LBS/HR, 0.040 LBS SOLUTE PER LB SOLVENT FEED
        0.90 LBS LIQUID PER LB SOLID IN UNDERFLOW

        BASIS 1 HOUR        V IN        L IN*       V OUT        L OUT*

        STAGE  1 OF  3
          TOTAL LBS        7000.0      2200.0      7580.0      1620.0
          LBS SOLVENT      6291.3         0.0      5183.4      1107.8
          LBS SOLUTE        708.7      2200.0      2396.6       512.2
          SOLUTE FRAC.      0.101       1.000       0.316       0.316

        STAGE  2 OF  3
          TOTAL LBS        7000.0      1620.0      7000.0      1620.0
          LBS SOLVENT      6639.4      1107.8      6291.3      1456.0
          LBS SOLUTE        360.6       512.2       708.7       164.0
          SOLUTE FRAC.      0.052       0.316       0.101       0.101

        STAGE  3 OF  3
          TOTAL LBS        7000.0      1620.0      7000.0      1620.0
          LBS SOLVENT      6720.0      1456.0      6639.4      1536.6
          LBS SOLUTE        280.0       164.0       360.6        83.4
          SOLUTE FRAC.      0.040       0.101       0.052       0.052

             * ALL L STREAMS ALSO CONTAIN  1800.0 LBS SOLID

          UNRECOVERED FRACTION OF TOTAL SOLUTE ENTERING = 0.034
```

b. Discussion of Results: For the one-, two-, and three-stage cases, the tabulated results show the oil mass fraction in the extract product stream to be 0.270, 0.308, and 0.316, respectively; and the fraction of total input oil lost in the raffinate is shown to be 0.177, 0.060, and 0.034, also respectively.

A comparison of these answers clearly shows the gain in both extract concentration and total oil recovered as the number of stages is increased. It is also apparent, however, that the gain per stage added diminishes as the total number of stages increases. This is readily demonstrable, if desired, by extending the calculations to cover additional stages.

As an example, increasing the number of stages to 20 only raises the oil concentration in the extract product stream to 0.319, and only lowers the fraction of total oil lost to 0.027. The results for the 20-stage case also show that the separation is essentially completed in the first six or seven stages, with negligible changes in compositions or quantities in the remaining stages.

The comparative results also make it clear that the total number of stages affects the conditions in any particular stage. For example, it can be seen that the results for the second stage of two stages clearly differ from those for the second stage of three stages. That this must necessarily be the case is not always obvious to students.

III. EDUCATIONAL (PEDAGOGICAL) ASPECTS

1. Description of Past Usage: This problem was originally developed for use in a sophomore-level stoichiometry course at Pratt Institute, its primary purpose being to develop the students' competence in computer programming. It was used in both semesters of the 1969-70 academic year. Further usage became impracticable when the author moved to the University of Arkansas, where stoichiometry students have not all had prior instruction in programming.

2. Concepts Demonstrated: a) The absorption-factor algorithm for multi-stage calculations; b) The advantages of countercurrent, multistage processes; c) The economic balance which dictates an optimum number of stages in view of the diminishing gain per additional stage added; d) Iterative-loop programming; e) Dimensioning and the use of subscripted variables.

3. Evaluation of Usage: Assignment of this problem was preceded by reading assignments and classroom discussion covering the general theory of countercurrent, multi-stage extraction, with emphasis on the pertinent mass balance calculations. The students then solved the one- and two-stage cases by slide-rule calculation, in a home assignment.

Discussion of the home assignment results was used to predict the increasing complexity of the calculations as the number of stages increases. The derivation of the absorption-factor equations was presented at this point, and attention was drawn to the iterative nature of the related calculations to set the stage for a computer solution. In the course of the discussion, the students were also shown a typical extrapolative technique and asked to predict the results for a three-stage process.

Two weeks were allowed for the writing, testing, debugging, and final execution of a computer solution to the problem, with other homework also assigned during this period. The students were encouraged to consult the instructor outside of class for any needed assistance, and most students responded to the invitation at least once before submitting their final programs and results.

All students completed the assignment, though the resulting programs differed considerably in level of sophistification and efficiency. While some of them almost certainly received outside assistance from other student programmers, it was quite apparent that all had improved their programming competence to a gratifying degree. The fact that many students, without coaching, extended their solutions to cover processes having four or more stages was also noteworthy.

A final discussion session was used to bring out or re-emphasize the several points presented under "Discussion of Results" (Sec. II-5b) herein. The liveliness of the discussion testified to the students' interest and personal involvement in the problem.

IV. PROGRAM SUMMARY SHEET

V. PROGRAM DESCRIPTION

1. General Description: The program structure is straightforward: The input data are read in, and the initial insolubles and total mass balances are completed, whereupon the value of the absorption-factor base number (AFB) is calculated. Vector values are then generated and stored for AFB raised to the Nth power (AFBN) and for the successive partial sums (SUM) of the series 1 + AFBN1 + AFBN2 + AFBN3 + ...

The next section of the program reads an input value for the number of stages (N), calculates the oil mass fraction in the extract product (Y2), and then iteratively calculates the oil mass fraction in each of the other streams. Mass fraction and total-mass values are then converted to input and output component masses and the results are output, stage by stage. A final section calculates and prints the fraction of total input oil lost in the raffinate product.

The program will handle N values ranging from 1 to 20, with execution terminated for any value outside this range. The output format provides for mass flow rates up to 99,999 pounds per hour. Otherwise, the program is essentially free of any limitations, assuming input data values to be realistic. It should be noted that the program does not provide for any limitation on solubility.

2. External Description: The program requires input data values for the feed rate (F), solute mass fraction in the feed (XF), solvent feed rate (V), solute mass fraction in the solvent feed (YN1), solution/solids ratio in the underflow streams (R), and the number of equilibrium stages (N). Rate values up to 99,999 are acceptable, with units of pounds per hour assumed in the output format.

Input N values may range from 1 to 20, and any number of N values may be processed in a single run. A final input N value of 0 should be used to terminate the run.

Input values for F, XF, V, YN1, and R are to be punched, in that order, into the first input data card under format (5F10.0). Successive input values for N are then punched on separate cards under format (I2). An echo print of the input data needed to run the one-, two-, and three-stage example problem is included with the tabulation of results presented under "Results" (Sec. II-5a) herein.

The printed output includes a statement of all input data specifications followed by a stage-by-stage listing of the calculated results. The Hollerith labels and line and column headings which accompany the output clearly denote the significance of each output value. Examples of the actual output format appear under "Results" (Sec. II-5a) herein.

3. Internal Description: The program logic is straightforward and is presumably adequately described in the foregoing "General Description" section and by the comments included in the program listing. With the exception of the provision for N values outside the permissible range of 1 to 20, the program contains no special error routines or related diagnostics.

Program Variables. Except as noted, the following program variables are real (floating-point) and unsubscripted, have the units of lbs/hr, and have a normal range of from 100 to 100,000 or so.

AFB	Absorption-Factor Base, dimensionless; range 0.2-5.
AFBN	AFB to nth power, dimensionless; DIMENSION 20; range 0 to 10^{14}
BI	Bottoms Liquid In
BLIQ	Bottoms Liquid
BSOL	Bottoms Solids
BXI	Bottoms Solvent In
BXO	Bottoms Solvent Out
BYI	Bottoms Solute In
BYO	Bottoms Solute Out
CON	Convenience Constant, dimensionless; range -1. to 1.
F	Feed
N	Number of Stages, integer, dimensionless; range 1 to 20
R	Ratio, solution-to-insolubles, dimensionless; range 0.5 to 2.
SLOSS	Solute Loss Fraction, dimensionless; range 0. to 0.5
SUM	Partial sums of 1 + AFBN1 + AFBN2 + AFBN3 + ..., dimensionless; DIMENSION 20; range 0 to 10^{14}
V	Solvent Feed and Overflow Liquid
VO	Overflow Liquid Out
VXI	Overflow Solvent In
VXO	Overflow Solvent Out

VYI	Overflow Solute In
VYO	Overflow Solute Out
V1	Extract Product
XF	Mass Fraction Solute in Feed, dimensionless; range 0 to 1
Y	Mass Fraction Solute, dimensionless; DIMENSION 22; range 0 to 1
YN1	Mass Fraction Solute in Solvent Feed, dimensionless; range 0 to 1

It should be noted that the program considers the N stages to be numbered from 2 through N+1. This permits the use of conventional nomenclature in which the subscript accompanying any variable denotes the stage in which the corresponding stream originates. Under this system, a zero subscript normally refers to the feed stream entering the first stage. The incremented stage numbering scheme used within the program avoids the problem of the zero subscript while still permitting the use of conventional nomenclature, since the feed stream subscript becomes one instead of zero.

VI. PROGRAM LISTING

```
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C                                                                        C
C  COUNTERCURRENT MULTI-STAGE SOLID-LIQUID EXTRACTION                    C
C                                                                        C
C  PROGRAM COMPLETED 20 DEC 69 BY C M THATCHER, DEPT OF CHEM ENGRG,      C
C    UNIV OF ARKANSAS, FAYETTEVILLE, ARKANSAS  72701                     C
C                                                                        C
C  PROGRAM USES ABSORPTION FACTOR METHOD TO CALCULATE THE COMPOSITION    C
C    AND QUANTITY OF ALL STREAMS FROM INPUT VALUES OF LB/HR OF FEED (F)  C
C    AND SOLUTE MASS FRACTION (XF), LB/HR OF SOLVENT (V) AND SOLUTE MASS C
C    FRACTION THEREIN (YN1), SOLUTION/SOLIDS RATIO IN UNDERFLOW STREAMS  C
C    (R), AND NUMBER OF EQUILIBRIUM STAGES (N).                          C
C                                                                        C
C  N RANGE IS FROM 1 TO 20, AND ANY NUMBER OF N VALUES MAY BE PROCESSED  C
C    IN A SINGLE RUN.  USE A FINAL INPUT N VALUE OF 0 TO TERMINATE THE   C
C    RUN.                                                                C
C                                                                        C
C  PUNCH INPUT VALUES FOR F, XF, V, YN1, AND R UNDER FORMAT (5F10.0).    C
C    PUNCH INPUT N VALUES ON SEPARATE CARDS UNDER FORMAT (I2).           C
C                                                                        C
C  NOTE THAT PROGRAM DOES NOT PROVIDE FOR A LIMITATION ON SOLUBILITY.    C
C                                                                        C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C
C  SET DIMENSIONS AND MACHINE-DEPENDENT I/O PARAMETERS.  (Y DIMENSIONED
C    FOR STAGES NUMBERED FROM 2--FEED STAGE--THROUGH N+2 TO AVOID ZERO
C    SUBSCRIPT.)
C
      DIMENSION Y(22), AFBN(20), SUM(20)
      INP = 5
      IOUT = 6
```

```
C
C  READ INPUT VALUES AND MAKE OVERALL BALANCE CALCULATIONS
C
      READ (INP,100) F, XF, V, YN1, R
      Y(1) = 1.
      BSOL = F*(1. - XF)
      BLIQ = R*BSOL
      AFB = BLIQ/V
      V1 = F*XF + V - BLIQ
C
C  GENERATE VECTORS FOR AFBN = AFB TO NTH POWER AND FOR SUCCESSIVE PARTIAL
C    SUMS OF SUM = 1 + AFBN1 + AFBN2 + AFBN3 + ...
C
      AFBN(1) = AFB
      SUM(1) = 1.
      DO 10 N = 1,19
      SUM(N+1) = SUM(N) + AFBN(N)
   10 AFBN(N+1) = AFB*AFBN(N)
C
C READ INPUT N VALUE, PRINT HEADINGS, CALCULATE Y VALUES
C
   20 READ (INP,101) N
      IF (N.LE.0.OR.N.GT.20) CALL EXIT
      WRITE (IOUT,102) F, XF, V, YN1, R
      Y(2) = (V*YN1 + F*XF*SUM(N))/(V*AFBN(N) + V1*SUM(N))
      IF (N.EQ.1) GO TO 40
      CON = (V1*Y(2) - F*XF)/V
      DO 30 J = 2,N
   30 Y(J+1) = AFBN(J-1)*Y(2) + SUM(J-1)*CON
   40 Y(N+2) = YN1
C
```

```
C COMPLETE CALCULATIONS AND PRINT RESULTS, STAGE BY STAGE
C
    VO = V1
    BI = F*XF
    DO 60 J = 1,N
    IF (J.NE.2) GO TO 50
    VO = V
    BI = BLIQ
  50 VYI = V*Y(J+2)
    VYO = VO*Y(J+1)
    BYI = BI*Y(J)
    BYO = BLIQ*Y(J+1)
    VXI = V - VYI
    VXO = VO - VYO
    BXI = BI - BYI
    BXO = BLIQ - BYO
  60 WRITE (IOUT,103) J, N, V, BI, VO, BLIQ, VXI, BXI, VXO, BXO,
   1  VYI, BYI, VYO, BYO, Y(J+2), Y(J), Y(J+1), Y(J+1)
C
C CALCULATE AND PRINT SOLUTE LOSS, WITH FOOTNOTE RE UNDERFLOW SOLIDS
C
    SLOSS = BLIQ*Y(N+1)/(F*XF + V*YN1) + 0.0005
    WRITE (IOUT,104) BSOL, SLOSS
    GO TO 20
C
C FORMAT STATEMENTS
C
 100 FORMAT (5F10.0)
 101 FORMAT (I2)
 102 FORMAT (1H1,18X,36HMASS BALANCE, MULTI-STAGE EXTRACTION///15H GIVE
   1N   FEED =,F7.0,8H LBS/HR,,F6.3,23H LBS SOLUTE PER LB FEED/9X,
   2 14HSOLVENT FEED =,F7.0,8H LBS/HR,,F6.3,31H LBS SOLUTE PER LB SOLV
   3ENT FEED/8X,F5.2,37H LBS LIQUID PER LB SOLID IN UNDERFLOW//9X,
   4 12HBASIS 1 HOUR,6X,4HV IN,6X,5HL IN*,6X,5HV OUT,6X,6HL OUT*/)
 103 FORMAT (9X,5HSTAGE,I3,3H OF,I3/11X,9HTOTAL LBS,F12.1,3F11.1/11X,
   1 11HLBS SOLVENT,F10.1,3F11.1/11X,10HLBS SOLUTE,4F11.1/11X,
   2 12HSOLUTE FRAC.,F9.3,3F11.3/)
 104 FORMAT (14X,28H* ALL L STREAMS ALSO CONTAIN,F8.1,10H LBS SOLID//
   1 11X,47HUNRECOVERED FRACTION OF TOTAL SOLUTE ENTERING =,F6.3///)
    END
```

I. PROBLEM IDENTIFICATION

1. Title: Liquid-Liquid Extraction
2. Author: Edward C. Roche, Jr.
3. Affiliation: Newark College of Engineering

II. TECHNICAL DESCRIPTION

1. Problem Statement:

The separation of a normal heptane-cyclohexane mixture is to be effected using furfural as the solvent. Laboratory test data on the three component system yielded the equilibrium compositions as tabulated in Table #1. An analysis of the experimental data was made using a non-linear regression procedure developed by Mr. R. Techo and resulted in the equilibrium data being adequately represented by the four-suffix Margules equation for a ternary system, the coefficients for which are tabulated in Table #2.

Preliminary process calculations which have been confirmed by laboratory test data indicate that a conventional end-feed column will yield satisfactory results. The results of the preliminary process calculations are tabulated in Table #3 in the form of guide lines for the separation of a normal heptana-cyclohexane feed.

Table #1

Laboratory Equilibrium Test Data

Hydrocarbon Rich Phase			Solvent Rich Phase		
Furfural	N-C_7	Cyclo-C_6	Furfural	N-C_7	Cyclo-C_6
.063	.187	.750	.871	.016	.113
.063	.222	.715	.875	.018	.106
.063	.247	.690	.877	.020	.102
.062	.311	.627	.884	.025	.091
.062	.416	.522	.894	.032	.074
.061	.496	.443	.901	.037	.062
.060	.592	.348	.910	.042	.048
.059	.698	.243	.919	.048	.033
.059	.797	.144	.928	.053	.019
.058	.834	.108	.931	.055	.014
.058	.865	.077	.933	.056	.010
.057	.908	.035	.937	.058	.004
.057	.922	.021	.938	.059	.003

Note: (1) Experimental data obtained at 30°C

(2) Compositions are mole fractions

Table #2

Four-Suffix Margules Equation

The Margules equation and the appropriate values for the 15 constants are tabulated below. The equation is written for component 4, but a by cyclic permutation of the subscripts the remaining equations are obtained.

$$\begin{aligned}\log_{10}\gamma_1 = {} & Z_2^2\,[A_{12} + 2Z_1(A_{21} - A_{12})] \\ & + Z_3^2\,[A_{13} + 2Z_1(A_{31} - A_{13})] \\ & + Z_2Z_3[A_{21} + A_{13} - A_{32} + 2Z_1(A_{31} - A_{13}) \\ & \qquad + 2Z_3(A_{32} - A_{23})] \\ & + Z_1Z_2^2(3Z_1-2)D_{12} + 3Z_2^2\,Z_3^2\,D_{23} \\ & + Z_1Z_3^2\,(2Z_1-2)D_{31} + Z_1Z_2Z_3\,(2-3Z_1)\,C_1 \\ & - Z_2^2\,Z_3(1-3Z_1)C_2 - Z_2Z_3^2\,(1-3Z_1)\,C_3\end{aligned}$$

Equation constants

1- Furfural
2- Normal heptane
3- Cyclohexane

*Binary Constants

$A_{11} = 0.0$ $A_{12} = 1.376$ $A_{13} = 1.345$

$A_{21} = 1.357$ $A_{22} = 0.0$ $A_{23} = 0.0$

$A_{31} = 1.016$ $A_{32} = 0.0$ $A_{33} = 0.0$

$D_{12} = 0.0$ $D_{23} = 0.0$ $D_{31} = 0.0$

*Ternary Constants

$C_1 = 0.0$ $C_2 = 0.0$ $C_3 = 0.0$

Table #3

Preliminary Process Design Summary

Hydrocarbon feed:

	moles/hour
Normal heptane	20.0
Cyclohexane	80.0
	100.0

Solvent:

Furfural (100% pure) is available as a solvent. A solvent-to-hydrocarbon feed ratio of 4.0 to 10.0 was found to give satisfactory results.

Specification:

The raffinate product is to contain no more than 0.010 mole fraction cyclohexane in a heptane-cyclohexane binary mixture.

II. TECHNICAL DESCRIPTION (Cont'd)

2. Problem Formulation and Technical Analysis:

Verify that the laboratory data is adequately represented by the four suffix Margules equation and the associated equation constant as given in Table #2.

Prepare a preliminary process design encompassing a conventional end-fed liquid-liquid extraction column. The preliminary design is to consist of a graphical solution of the appropriate stagewise problem with no attempt at obtaining a consistent number of theoretical contact stages and solvent feed rate.

With the design parameters established via the preliminary design verification as well as finalization of the process design can be accomplished using the digital simulation program.

3. Method of Solution:

The verification of the laboratory data as given in Table #2 is accomplished by using the activity coefficient as defined by the four suffix Margules equation to generate compotential activity data for each component for each pair of raffinate (hydrocarbon rich) - extract (solvent rich) data. Comparison of the componential activity data will verify the validity of the given laboratory data.

The preliminary process design was accomplished on both a triangular phase diagram, and also on the solvent free phase diagram. A solvent rate was assumed that would result in the overall column mixing point located in the two phase region and also would not result in a "pinch-point" within the column itself due to insufficient solvent. The preliminary design made no attempt at obtaining a solvent feed rate and number of theoretical contact stages consistent with the given raffinate product specification.

4. Input Required to Simulation Program:

The program input data is specified by the attached user's manual which contains the program description outlining the card sequence and card content.

5. References:

British Chem. Eng. Rigorous Solution of Multicomponent Multistage liquid-liquid extraction problems, by E.C. Roche, Vol. 14, No. 10, pg. 1393 (Oct. 1969)

British Chem. Eng., General Design Algorithm for Multistage Countercurrent Equilibrium Processes, by E.C. Roche, Jr., Vol. 16, No. 9, pg. 821 (Sept. 1971)

II. TECHNICAL DESCRIPTION (Cont'd)

6. Solution:

The solution to the liquid-liquid extraction problem is contained in the attached computer printout which summarizes the input and the converged solution to the stagewise problem.

III. EDUCATIONAL ASPECTS

1. Description of Past Usage:

This program and the process problem contained in this writeup were used by approximately 40 students in the senior design course required of all students. The overall results of this process oriented design problem were excellent.

2. Concepts Demonstrated:

The following objectives were attained as part of the process design problem: (1) multiplicity of valid solutions to the problem; (2) proper role of computer simulation models in solving process problems, and (3) the interrelationships between the process design variables.

3. Evaluation of Usage:

The liquid-liquid extraction problem was covered as a three week assignment. Student interest can be maintained by altering one or more of the following: (1) hydrocarbon feed composition, (2) solvent feed composition, and (3) raffinate product specification.

4. Nature of Assignments:

The specific assignments to the students were: (1) verify the laboratory data, (2) prepare a preliminary process design, and (3) verify and finalize the process design using the simulation program.

IV. PROGRAM SUMMARY SHEET

The program summary sheet for the liquid-liquid extraction program is included with CACHE submission attachments.

V. PROGRAM DESCRIPTION

1. Program Description:

The functional purpose of the main onroot program LIQLIQ is to control the computational sequence of the problem as well as control over the intermediate print out. The subprogram IQ handles the basic problem input along with the final overall material balance summary. The solution of the linearized material balance and equilibrium stagewise equations are solved by the editorial subprogram MATRIX. The entries into the coefficient matrix and right hand sides is performed by ABCD, with equilibrium data being supplied by ACTO. Utility rou-

V. PROGRAM DESCRIPTION (Cont'd)

1. Program Description (Cont'd)

tines used by the stagewise model are SPINV, CLEAR, and PUNCH

2. External and Internal Description:

The main program and the associated subprograms contain via comment cards descriptive information on the program functions and specific variable definitions. The formulation of the input data is covered by the User's Manual which is included as an attachment.

Program diagnostics are provided to specify incomplete problem formulation. There is no check made by the program as to feasibility such as for a fixed hydrocarbon-solvent feed rate yielding a single phase system.

3. Program Listing:

A listing of the program source cards is included as an attachment.

USER'S MANUAL

LIQLIQ

RIGOROUS LIQUID-LIQUID EXTRACTION PROGRAM
(Four-suffix Margules Equation for a Ternary System)

PROGRAM LIQLIQ

Introduction

Program LIQLIQ is a rigorous liquid-liquid extraction program written in FORTRAN IV capable of handling a column of up to 30 contact stages. The program is capable of handling a solvent recovery system coupled with extract reflux, which when invoked is taken as stage #1.

The program is capable of solving the general liquid-liquid extraction problem having a maximum of 9 components, up to 7 feeds, and up to 5 sidestreams (raffinate and/or extract).

The method of solution is that of the general Newton-Raphson procedure for solving a set of non-linear equations simultaneously. The method is applied repeatedly until all of the problem constraints are satisfied. Included in the constraint set is the provision to converge to either a stream rate or composition by adjusting as a control variable a specific feed stream.

Program LIQLIQ is limited to 3 components due to the activity coefficient expression that is incorporated in the model. LIQLIQ utilizes the four-suffix Margules equation for a ternary system. The basic program can handle up to 9 components, but the activity coefficient module must be replaced to reflect the appropriate expression.

Card Sequence and Content

1. Title card, columns 2-80
   Three title cards must be supplied with each problem and may contain any descriptive information desired.

2. Control card

   All data on this card must be punched within the specified space right justified.

   a. Columns 1-4 Number of contact stages ($1 \leq N \leq 30$)

   b. Columns 5-8 Number of components (LIQLIQ is designed for 3 components)

   c. Columns 9-12 Code for extract reflux (0= No, 1= Yes)

   d. Columns 13-16 Number of feed streams ($1 \leq F \leq 7$)

   e. Columns 17-20 Number of raffinate sidestreams ($0 \leq SS \leq 5$)

   f. Columns 21-24 Number of extract sidestreams ($0 \leq SS \leq 5$)

   g. Columns 25-28 All internal stream rates available as input data (0=No, 1=Yes)

   h. Columns 29-32 All internal stream compositions available as input data (0=No, 1=Yes)

   i. Columns 33-36 Maximum number of iterations (If no value is entered 20 will be used)

   j. Columns 37-40 Print Code

      1 Input plus converged case
      2 1 + Summary of all iterations
      3 2 + compositions and rates for each iteration

   k. Columns 41-44 Number of design specifications ($0 \leq \text{Spec} \leq 4$)

   l. Columns 45-48 Punch option - punched cards containing internal stream rates and compositions can be obtained at the end of the specified number of iterations to facilitate problem restart (0=No, 1=Yes).

3. Tolerances for convergence test

   a. Columns 1-8 Composition test (A reasonable value for $\frac{\Delta x}{x}$ and $\frac{\Delta y}{y}$ is 0.005)

   b. Columns 9-16 Flow test (A reasonable value for $\frac{\Delta L}{L}$ and $\frac{\Delta V}{V}$ is 0.005)

   c. Columns 17-24 Flow rate change limit. (If no value is entered 0.50 is assumed).

4. Input streams

For each feed stream one data card is supplied containing the componential flow rates for component 1, component 2, component 3, etc., in the order specified on the stage number card.

a. Columns 1-4, 5-8, 9-12, etc. Enter the stage number for the feed streams right justified in the order that the flow rates are to be entered.

b. Columns 1-8, 9-16, 17-24, etc. Componential flow rates for the first feed; component 1, component 2, component 3, etc.

c. Columns 1-8, 9-16, 17, 24, etc. Componential flow rates for the second feed; component 1, component 2, component 3, etc.

5. Raffinate side streams

If the raffinate side stream code is zero (0) the following data cards are to be omitted.

a. Columns 1-4, 5-8, 9-12, etc. Enter the stage number for the sidestream (raffinate) right justified in the order that the flow rates are entered.

b. Columns 1-8, 9-16, 17-24, etc. Raffinate sidestream flow rate 1, sidestream flow rate 2, etc.

6. Extract Sidestreams

If the extract sidestream code is zero (0) the following data cards are to be omitted.

a. Columns 1-4, 5-8, 9-12, etc. Enter the stage number for the sidestream (extract) right justified in the order that the flow rates are entered.

b. Columns 1-8, 9-16, 17-24 etc. Raffinate sidestream flow rate 1, sidestream flow rate 2, etc.

7. Data for extract reflux - solvent recovery system.

If the extract reflux code is zero (0) the following data cards are to be omitted.

a. Columns 1-8 Extract reflux ratio. (This number is defined as the ratio of the net raffinate to stage 2 divided by the extract product.

b. Columns 1-8, 9-16, 17-24, etc. Componential recoveries accomplished by the solvent recovery system entered in the same componential order used in specifying the feed streams. (The recovery is entered as a fraction and is defined as V_1y_i/V_2y_i with V_1 being the recovered solvent and V_2 being the extract leaving stage 2).

8. Internal Stream Rates Definition

Two forms of internal flow stream definition are available and are described as follows:

a. The internal stream rates availability code must be equal to 1 (control card item g)

   (1) First set of cards contains the raffinate flow rates, 9 values per card with as many cards as are required. Column 1-8, 9-16, 17-24, etc. Raffinate flow rate from stage 1, stage 2, stage 3, etc.

   (2) Second set of cards contains the extract flow rates, 9 values per card with as many cards as are required. Column 1-8, 9-16, 17-24, etc. Extract flow rate from stage 1, stage 2, stage 3, etc.

   Note: This form of input has been designed to be compatable with the punch option available within the program.

b. The internal stream rates availability code must be equal to 0 (control card item g). Under this option the program generates an initial set of flow rates using the feed and side stream data.

   Note: No data cards are required.

9. Internal Stream Compositions Definition

Two forms of internal stream compositions definition are available and are described as follows:

a. The internal stream composition availability code must be equal to 1 (control card item h).

   (1) First set of cards contains the raffinate compositions, one card per stage with each card containing the compositional values. Columns 1-8, 9-16, 17-24, etc. component 1, component 2, component 3, etc.

   (2) Second set of cards contains the extract compositions, one card per stage with each card containing the compositional values. Columns 1-8, 9-16, 17-24, etc. Component 1, component 2, component 3, etc.

b. The internal stream composition availability code must be equal to 0 (control card item h)

   (1) First set of 2 cards inputs the first and last raffinate stages compositional values. Columns 1-8, 9-16, 17-24, etc. component 1, component 2, component 3, etc.

   (2) Second set of 2 cards inputs the first and last extract stages compositional values. Columns 1-8, 9-16, 17-24, etc. component 1, component 2, component 3, etc.

   Note: The program will take the above data and generate the missing values via linear interpolation.

10. Specification Information

The following information is to be supplied only if the number of problem specifications is greater than 0 (control card item k). The number of contact stages is not a control variable. For each specification one card containing the following data is to be supplied:

a. Columns 1-8	Code for type of specification - data must be right justified 1 Raffinate rate }For this specification 2 Extract rate }item b is to be ignored 3 Raffinate composition 4 Extract composition
b. Columns 9-16	Stage on which specification is located - data must be right justified
c. Columns 17-24	Component on which specification is given - data must be right justified
d. Columns 25-32	Numeric value of specifications
e. Columns 33-40	Control parameter designation, that is, the feed number as inputed- data must be right justified.

11. Activity Coefficient Data

The following describes how one inputs the constants for the four suffix Margules equation for a ternary system.

All data is inputed using Columns 1-8, 9-16, and 17-24.

a. Card 1: A_{11}, A_{12}, and A_{13}
b. Card 2: A_{12}, A_{22}, and A_{23}
c. Card 3: A_{31}, A_{32}, and A_{33}
d. Card 3: D_{12}, D_{23}, and D_{31}
e. Card 4: C_1, C_2, and C_3

COMPUTER OUTPUT FOR
PROCESS DESIGN PROBLEM

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```
CHE 70 COURSE PROBLEM  **  SPEC IS ON RAFFINATE PRODUCT, COMP # 3
COMPONENTS    (1) FURFURAL      (2) NORMAL HEPTANE      (3) CYCLOHEXANE
                  SOLVENT           DILUENT                 SOLUTE


TOTAL NUMBER OF STAGES   12
NUMBER OF COMPONENTS      3
EXTRACT REFLUX CODE       0
NUMBER OF SPECIFICATIONS  1


TOLERANCES ON COMPUTED VARIABLES
    COMPOSITIONS 0.005000
    FLOW RATES   0.005000

MAXIMUM FRACTIONAL CHANGE IN FLOW RATES PER ITERATION  0.200000


NUMBER OF FEED STREAMS    2
SOLVENT FEED IS           2

FEED     STAGE
   1         1
   2        12

COMP          FD 1         FD 2
   1         0.000      650.000
   2        20.000        0.000
   3        80.000        0.000
 TOT       100.000      650.000


DESIGN SPECIFICATION OPTIONS

NO  TYPE  STAGE  COMP NO  SPEC VALUE  CONTROL
 1     3     12        3  1.0000E-02        2
```

```
ITERATION NUMBER      0


DESCRIPTION                 STAGE          RATE
RAFFINATE PRODUCT             12          10.000
EXTRACT PRODUCT                1         745.000


STAGE         RAF RATE         EXT RATE
  1           105.000          745.000
  2           100.000          740.000
  3            95.000          735.000
  4            90.000          730.000
  5            85.000          725.000
  6            80.000          720.000
  7            75.000          715.000
  8            70.000          710.000
  9            65.000          705.000
 10            60.000          700.000
 11            55.000          700.000
 12            10.000          700.000


STAGE NUMBER        1

COMP          RAF FRAC         EXT FRAC          RAF RATE          EXT RATE
  1          0.0600000        0.8700000            6.300           648.150
  2          0.2200000        0.0200000           23.100            14.900
  3          0.7200000        0.1100000           75.600            81.950
 TOT         1.0000000        1.0000000          105.000           745.000


STAGE NUMBER        2

COMP          RAF FRAC         EXT FRAC          RAF RATE          EXT RATE
  1          0.0600000        0.8763636            6.000           648.509
  2          0.2781818        0.0236364           27.818            17.491
  3          0.6618182        0.1009091           66.182            74.673
 TOT         0.9999999        1.0009089          100.000           740.000


STAGE NUMBER        3

COMP          RAF FRAC         EXT FRAC          RAF RATE          EXT RATE
  1          0.0600000        0.8827273            5.700           648.804
  2          0.3363636        0.0272727           31.955            20.045
  3          0.6036364        0.0918181           57.345            67.486
 TOT         0.9999999        1.0018177           95.000           735.000
```

```
STAGE NUMBER        4

COMP        RAF FRAC        EXT FRAC        RAF RATE        EXT RATE
   1       0.0600000       0.8890909           5.400         649.036
   2       0.3945453       0.0309091          35.509          22.564
   3       0.5454546       0.0827271          49.091          60.391
 TOT       0.9999998       1.0027266          90.000         730.000

STAGE NUMBER        5

COMP        RAF FRAC        EXT FRAC        RAF RATE        EXT RATE
   1       0.0600000       0.8954545           5.100         649.204
   2       0.4527271       0.0345454          38.482          25.045
   3       0.4872727       0.0736362          41.418          53.386
 TOT       0.9999998       1.0036354          85.000         725.000

STAGE NUMBER        6

COMP        RAF FRAC        EXT FRAC        RAF RATE        EXT RATE
   1       0.0600000       0.9018182           4.800         649.309
   2       0.5109088       0.0381818          40.873          27.491
   3       0.4290909       0.0645452          34.327          46.473
 TOT       0.9999997       1.0045443          80.000         720.000

STAGE NUMBER        7

COMP        RAF FRAC        EXT FRAC        RAF RATE        EXT RATE
   1       0.0600000       0.9081818           4.500         649.350
   2       0.5690906       0.0418182          42.682          29.900
   3       0.3709091       0.0554543          27.818          39.650
 TOT       0.9999996       1.0054541          75.000         715.000

STAGE NUMBER        8

COMP        RAF FRAC        EXT FRAC        RAF RATE        EXT RATE
   1       0.0600000       0.9145454           4.200         649.327
   2       0.6272724       0.0454545          43.909          32.273
   3       0.3127273       0.0463634          21.891          32.918
 TOT       0.9999996       1.0063629          70.000         710.000
```

```
STAGE NUMBER        9

COMP          RAF FRAC          EXT FRAC          RAF RATE          EXT RATE
   1         0.0600000         0.9209090             3.900           649.241
   2         0.6854541         0.0490909            44.555            34.609
   3         0.2545455         0.0372725            16.545            26.277
 TOT         0.9999995         1.0072718            65.000           705.000

STAGE NUMBER       10

COMP          RAF FRAC          EXT FRAC          RAF RATE          EXT RATE
   1         0.0600000         0.9272727             3.600           649.091
   2         0.7436359         0.0527272            44.618            36.909
   3         0.1963636         0.0281816            11.782            19.727
 TOT         0.9999995         1.0081806            60.000           700.000

STAGE NUMBER       11

COMP          RAF FRAC          EXT FRAC          RAF RATE          EXT RATE
   1         0.0600000         0.9336363             3.300           653.545
   2         0.8018177         0.0563636            44.100            39.455
   3         0.1381818         0.0190907             7.600            13.363
 TOT         0.9999994         1.0090904            55.000           700.000

STAGE NUMBER       12

COMP          RAF FRAC          EXT FRAC          RAF RATE          EXT RATE
   1         0.0600000         0.9400000             0.600           658.000
   2         0.8600000         0.0600000             8.600            42.000
   3         0.0800000         0.0100000             0.800             7.000
 TOT         0.9999999         1.0099993            10.000           700.000
```

```
ITERATION NUMBER     1

DESCRIPTION                   STAGE          RATE
RAFFINATE PRODUCT               12          8.000
EXTRACT PRODUCT                  1        743.112

STAGE        RAF RATE        EXT RATE
  1          104.650         743.112
  2           98.597         747.762
  3           91.571         741.709
  4           83.738         734.684
  5           75.546         726.850
  6           67.645         718.659
  7           60.736         710.757
  8           56.000         703.848
  9           52.000         698.505
 10           50.135         695.010
 11           49.746         693.247
 12            8.000         692.858

STAGE NUMBER          1

COMP         RAF FRAC        EXT FRAC        RAF RATE        EXT RATE
  1         0.0620960       0.8745970           6.498         649.924
  2         0.2156992       0.0175491          22.573          13.041
  3         0.7222047       0.1078574          75.578          80.150
 TOT        0.9999999       1.0000029         104.650         743.112

STAGE NUMBER          2

COMP         RAF FRAC        EXT FRAC        RAF RATE        EXT RATE
  1         0.0574160       0.8778855           5.661         656.449
  2         0.2587619       0.0208437          25.513          15.586
  3         0.6838220       0.1012740          67.423          75.729
 TOT        0.9999999       1.0000029          98.597         747.762

STAGE NUMBER          3

COMP         RAF FRAC        EXT FRAC        RAF RATE        EXT RATE
  1         0.0588579       0.8839152           5.390         655.608
  2         0.3168294       0.0249519          29.012          18.507
  3         0.6243126       0.0911359          57.169          67.596
 TOT        0.9999999       1.0000029          91.571         741.709
```

```
STAGE NUMBER        4

COMP         RAF FRAC        EXT FRAC        RAF RATE      EXT RATE
  1         0.0616228       0.8920067          5.160        655.343
  2         0.3923055       0.0299143         32.851         21.978
  3         0.5460717       0.0780818         45.727         57.365
 TOT        0.9999999       1.0000019         83.738        734.684

STAGE NUMBER        5

COMP         RAF FRAC        EXT FRAC        RAF RATE      EXT RATE
  1         0.0616800       0.9013119          4.660        655.119
  2         0.4847174       0.0355993         36.619         25.875
  3         0.4536028       0.0630913         34.268         45.858
 TOT        1.0000000       1.0000019         75.546        726.850

STAGE NUMBER        6

COMP         RAF FRAC        EXT FRAC        RAF RATE      EXT RATE
  1         0.0564953       0.9108488          3.822        654.589
  2         0.5896762       0.0416783         39.888         29.952
  3         0.3538287       0.0474751         23.935         34.118
 TOT        1.0000000       1.0000019         67.645        718.659

STAGE NUMBER        7

COMP         RAF FRAC        EXT FRAC        RAF RATE      EXT RATE
  1         0.0457440       0.9196389          2.778        653.640
  2         0.6987936       0.0476567         42.442         33.872
  3         0.2554626       0.0327062         15.516         23.246
 TOT        1.0000000       1.0000010         60.736        710.757

STAGE NUMBER        8

COMP         RAF FRAC        EXT FRAC        RAF RATE      EXT RATE
  1         0.0315701       0.9268965          1.768        652.394
  2         0.8009281       0.0529664         44.852         37.280
  3         0.1675022       0.0201387          9.380         14.175
 TOT        1.0000000       1.0000010         56.000        703.848
```

```
STAGE NUMBER         9

COMP          RAF FRAC        EXT FRAC        RAF RATE      EXT RATE
   1         0.0180886       0.9322025           0.941       651.148
   2         0.8846793       0.0570993          46.003        39.884
   3         0.0972324       0.0106999           5.056         7.474
 TOT         1.0000000       1.0000010          52.000       698.505

STAGE NUMBER        10

COMP          RAF FRAC        EXT FRAC        RAF RATE      EXT RATE
   1         0.0101521       0.9355861           0.509       650.241
   2         0.9414220       0.0597430          47.198        41.522
   3         0.0484259       0.0046720           2.428         3.247
 TOT         1.0000000       1.0000010          50.135       695.010

STAGE NUMBER        11

COMP          RAF FRAC        EXT FRAC        RAF RATE      EXT RATE
   1         0.0121281       0.9374226           0.603       649.865
   2         0.9665595       0.0608038          48.083        42.152
   3         0.0213124       0.0017745           1.060         1.230
 TOT         1.0000000       1.0000000          49.746       693.247

STAGE NUMBER        12

COMP          RAF FRAC        EXT FRAC        RAF RATE      EXT RATE
   1         0.0256675       0.9384696           0.205       650.226
   2         0.9640321       0.0605840           7.712        41.976
   3         0.0103006       0.0009470           0.082         0.656
 TOT         1.0000000       1.0000000           8.000       692.858
```

```
ITERATION NUMBER     2

DESCRIPTION                    STAGE           RATE
RAFFINATE PRODUCT               12            7.330
EXTRACT PRODUCT                  1          742.672

STAGE          RAF RATE        EXT RATE
   1            103.595         742.672
   2             98.210         746.267
   3             91.312         740.882
   4             83.413         733.983
   5             75.342         726.084
   6             68.063         718.013
   7             62.292         710.733
   8             58.182         704.962
   9             55.301         700.852
  10             53.266         697.971
  11             52.063         695.936
  12              7.330         694.732

STAGE NUMBER          1

COMP          RAF FRAC        EXT FRAC         RAF RATE       EXT RATE
   1         0.0638366       0.8746778          6.613         649.598
   2         0.2167200       0.0177901         22.451          13.212
   3         0.7194434       0.1075326         74.531          79.861
  TOT        0.9999999       1.0000000        103.595         742.672

STAGE NUMBER          2

COMP          RAF FRAC        EXT FRAC         RAF RATE       EXT RATE
   1         0.0646551       0.8793252          6.350         656.211
   2         0.2607301       0.0209903         25.606          15.664
   3         0.6746148       0.0996851         66.254          74.392
  TOT        1.0000000       1.0000000         98.210         746.267

STAGE NUMBER          3

COMP          RAF FRAC        EXT FRAC         RAF RATE       EXT RATE
   1         0.0642108       0.8853638          5.863         655.950
   2         0.3228262       0.0254008         29.478          18.819
   3         0.6129630       0.0892358         55.971          66.113
  TOT        1.0000000       1.0000000         91.312         740.882
```

```
STAGE NUMBER         4

COMP         RAF FRAC        EXT FRAC        RAF RATE        EXT RATE
   1        0.0629838       0.8930204          5.254         655.462
   2        0.4044173       0.0309150         33.734          22.691
   3        0.5325989       0.0760652         44.426          55.831
 TOT        0.9999999       1.0000000         83.413         733.983

STAGE NUMBER         5

COMP         RAF FRAC        EXT FRAC        RAF RATE        EXT RATE
   1        0.0606190       0.9018955          4.567         654.852
   2        0.5025516       0.0371151         37.863          26.949
   3        0.4368295       0.0609903         32.912          44.284
 TOT        1.0000000       1.0000000         75.342         726.084

STAGE NUMBER         6

COMP         RAF FRAC        EXT FRAC        RAF RATE        EXT RATE
   1        0.0575874       0.9110764          3.920         654.165
   2        0.6077877       0.0432838         41.368          31.078
   3        0.3346251       0.0456410         22.775          32.771
 TOT        1.0000000       1.0000010         68.063         718.013

STAGE NUMBER         7

COMP         RAF FRAC        EXT FRAC        RAF RATE        EXT RATE
   1        0.0550687       0.9194967          3.430         653.516
   2        0.7063947       0.0486432         44.002          34.572
   3        0.2385368       0.0318611         14.859          22.645
 TOT        1.0000000       1.0000000         62.292         710.733

STAGE NUMBER         8

COMP         RAF FRAC        EXT FRAC        RAF RATE        EXT RATE
   1        0.0526823       0.9263089          3.065         653.012
   2        0.7880487       0.0527727         45.850          37.203
   3        0.1592693       0.0209193          9.267          14.747
 TOT        1.0000000       1.0000000         58.182         704.962
```

```
STAGE NUMBER          9

COMP         RAF FRAC        EXT FRAC        RAF RATE        EXT RATE
   1        0.0489997       0.9311720           2.710         652.614
   2        0.8503810       0.0557714          47.027          39.087
   3        0.1006194       0.0130574           5.564           9.151
 TOT        1.0000000       1.0000000          55.301         700.852

STAGE NUMBER         10

COMP         RAF FRAC        EXT FRAC        RAF RATE        EXT RATE
   1        0.0457047       0.9344235           2.434         652.201
   2        0.8939404       0.0578062          47.616          40.347
   3        0.0603549       0.0077706           3.215           5.424
 TOT        0.9999999       1.0000000          53.266         697.971

STAGE NUMBER         11

COMP         RAF FRAC        EXT FRAC        RAF RATE        EXT RATE
   1        0.0467964       0.9367499           2.436         651.918
   2        0.9190266       0.0588735          47.847          40.972
   3        0.0341770       0.0043764           1.779           3.046
 TOT        0.9999999       0.9999999          52.063         695.936

STAGE NUMBER         12

COMP         RAF FRAC        EXT FRAC        RAF RATE        EXT RATE
   1        0.0526045       0.9384224           0.386         651.952
   2        0.9291881       0.0592557           6.811          41.167
   3        0.0182077       0.0023223           0.133           1.613
 TOT        1.0000000       1.0000000           7.330         694.732
```

(Printout of iterations 3-12 is omitted for compactness)

```
ITERATION NUMBER    13


DESCRIPTION                   STAGE          RATE
RAFFINATE PRODUCT              12            6.031
EXTRACT PRODUCT                 1          760.305


STAGE          RAF RATE        EXT RATE
   1           101.860         760.305
   2            94.236         762.164
   3            85.402         754.541
   4            76.418         745.706
   5            68.475         736.721
   6            62.316         728.779
   7            58.024         722.620
   8            55.254         718.328
   9            53.557         715.558
  10            52.548         713.860
  11            51.961         712.852
  12             6.031         712.264


STAGE NUMBER          1

COMP          RAF FRAC        EXT FRAC         RAF RATE        EXT RATE
   1         0.0628495       0.8760006           6.402         666.028
   2         0.2317386       0.0189253          23.605          14.389
   3         0.7054118       0.1050722          71.853          79.887
  TOT        0.9999999       0.9999982         101.860         760.305


STAGE NUMBER          2

COMP          RAF FRAC        EXT FRAC         RAF RATE        EXT RATE
   1         0.0624560       0.8823043           5.886         672.461
   2         0.2959573       0.0235940          27.890          17.983
   3         0.6415867       0.0940995          60.461          71.719
  TOT        0.9999999       0.9999978          94.236         762.164


STAGE NUMBER          3

COMP          RAF FRAC        EXT FRAC         RAF RATE        EXT RATE
   1         0.0618736       0.8905677           5.284         671.969
   2         0.3818839       0.0294918          32.613          22.253
   3         0.5562425       0.0799384          47.504          60.317
  TOT        0.9999999       0.9999978          85.402         754.541
```

```
STAGE NUMBER        4

COMP        RAF FRAC        EXT FRAC         RAF RATE        EXT RATE
   1       0.0611002       0.9003386            4.669         671.388
   2       0.4861456       0.0361496           37.150          26.957
   3       0.4527543       0.0635102           34.598          47.360
 TOT       0.9999999       0.9999985           76.418         745.706

STAGE NUMBER        5

COMP        RAF FRAC        EXT FRAC         RAF RATE        EXT RATE
   1       0.0602033       0.9104922            4.122         670.779
   2       0.5977392       0.0427218           40.930          31.474
   3       0.3420575       0.0467841           23.422          34.467
 TOT       0.9999999       0.9999981           68.475         736.721

STAGE NUMBER        6

COMP        RAF FRAC        EXT FRAC         RAF RATE        EXT RATE
   1       0.0593188       0.9196532            3.697         670.224
   2       0.7013832       0.0483579           43.708          35.242
   3       0.2392979       0.0319875           14.912          23.312
 TOT       0.9999999       0.9999985           62.316         728.779

STAGE NUMBER        7

COMP        RAF FRAC        EXT FRAC         RAF RATE        EXT RATE
   1       0.0585729       0.9268743            3.399         669.778
   2       0.7851713       0.0526126           45.559          38.019
   3       0.1562558       0.0205115            9.067          14.822
 TOT       1.0000000       0.9999983           58.024         722.620

STAGE NUMBER        8

COMP        RAF FRAC        EXT FRAC         RAF RATE        EXT RATE
   1       0.0580187       0.9319659            3.206         669.457
   2       0.8453996       0.0555159           46.712          39.879
   3       0.0965817       0.0125165            5.337           8.991
 TOT       0.9999999       0.9999983           55.254         718.328
```

```
STAGE NUMBER        9

COMP          RAF FRAC        EXT FRAC        RAF RATE        EXT RATE
   1         0.0576440       0.9352742          3.087          669.243
   2         0.8850566       0.0573601         47.401           41.044
   3         0.0572995       0.0073640          3.069            5.269
 TOT         1.0000000       0.9999983         53.557          715.558

STAGE NUMBER       10

COMP          RAF FRAC        EXT FRAC        RAF RATE        EXT RATE
   1         0.0574072       0.9373093          3.017          669.108
   2         0.9096607       0.0584785         47.801           41.745
   3         0.0329321       0.0042106          1.731            3.006
 TOT         0.9999999       0.9999984         52.548          713.860

STAGE NUMBER       11

COMP          RAF FRAC        EXT FRAC        RAF RATE        EXT RATE
   1         0.0572643       0.9385191          2.976          669.025
   2         0.9243615       0.0591373         48.031           42.156
   3         0.0183742       0.0023421          0.955            1.670
 TOT         0.9999999       0.9999984         51.961          712.852

STAGE NUMBER       12

COMP          RAF FRAC        EXT FRAC        RAF RATE        EXT RATE
   1         0.0571801       0.9392234          0.345          668.975
   2         0.9329477       0.0595188          5.627           42.393
   3         0.0098722       0.0012561          0.060            0.895
 TOT         0.9999999       0.9999983          6.031          712.264
```

```
ITERATION NUMBER   14


DESCRIPTION                  STAGE          RATE
RAFFINATE PRODUCT             12           6.030
EXTRACT PRODUCT                1         760.307


STAGE         RAF RATE         EXT RATE
  1           101.855          760.307
  2            94.231          762.161
  3            85.397          754.537
  4            76.414          745.703
  5            68.475          736.720
  6            62.319          728.781
  7            58.027          722.625
  8            55.256          718.332
  9            53.556          715.561
 10            52.547          713.861
 11            51.960          712.851
 12             6.030          712.264


STAGE NUMBER         1

COMP          RAF FRAC         EXT FRAC          RAF RATE         EXT RATE
  1          0.0627255        0.8759499            6.389          665.990
  2          0.2314657        0.0189070           23.576           14.375
  3          0.7058087        0.1051413           71.890           79.940
 TOT         0.9999999        0.9999982          101.855          760.307

STAGE NUMBER         2

COMP          RAF FRAC         EXT FRAC          RAF RATE         EXT RATE
  1          0.0622641        0.8822011            5.867          672.379
  2          0.2953022        0.0235527           27.827           17.951
  3          0.6424336        0.0942446           60.537           71.830
 TOT         0.9999999        0.9999983           94.231          762.161

STAGE NUMBER         3

COMP          RAF FRAC         EXT FRAC          RAF RATE         EXT RATE
  1          0.0617382        0.8904229            5.272          671.857
  2          0.3807429        0.0294243           32.514           22.202
  3          0.5575188        0.0801510           47.610           60.477
 TOT         0.9999999        0.9999983           85.397          754.537
```

```
STAGE NUMBER        4

COMP        RAF FRAC        EXT FRAC        RAF RATE        EXT RATE
   1       0.0611493       0.9001737           4.673         671.262
   2       0.4845008       0.0360591          37.023          26.889
   3       0.4543498       0.0637655          34.719          67.550
 TOT       0.9999999       0.9999983          76.414         745.703

STAGE NUMBER        5

COMP        RAF FRAC        EXT FRAC        RAF RATE        EXT RATE
   1       0.0604882       0.9103359           4.142         670.662
   2       0.5957432       0.0426182          40.794          31.398
   3       0.3437685       0.0470441          23.540          34.658
 TOT       0.9999999       0.9999982          68.475         736.720

STAGE NUMBER        6

COMP        RAF FRAC        EXT FRAC        RAF RATE        EXT RATE
   1       0.0597661       0.9195241           3.725         670.131
   2       0.6993437       0.0482569          43.583          35.169
   3       0.2408901       0.0322173          15.012          23.479
 TOT       0.9999999       0.9999983          62.319         728.781

STAGE NUMBER        7

COMP        RAF FRAC        EXT FRAC        RAF RATE        EXT RATE
   1       0.0590459       0.9267795           3.426         669.713
   2       0.7833990       0.0525277          45.458          37.958
   3       0.1575550       0.0206910           9.142          14.952
 TOT       0.9999999       0.9999982          58.027         722.625

STAGE NUMBER        8

COMP        RAF FRAC        EXT FRAC        RAF RATE        EXT RATE
   1       0.0584158       0.9319021           3.228         669.415
   2       0.8440550       0.0554526          46.639          39.833
   3       0.0975292       0.0126433           5.389           9.082
 TOT       0.9999999       0.9999980          55.256         718.332
```

```
STAGE NUMBER        9

COMP        RAF FRAC         EXT FRAC          RAF RATE          EXT RATE
   1       0.0579314        0.9352335             3.103           669.216
   2       0.8841360        0.0573175            47.351            41.014
   3       0.0579327        0.0074470             3.103             5.329
 TOT       1.0000000        0.9999979            53.556           715.561


STAGE NUMBER       10

COMP        RAF FRAC         EXT FRAC          RAF RATE          EXT RATE
   1       0.0575955        0.9372851             3.026           669.091
   2       0.9090766        0.0584513            47.769            41.726
   3       0.0333280        0.0042618             1.751             3.042
 TOT       0.9999999        0.9999982            52.547           713.861


STAGE NUMBER       11

COMP        RAF FRAC         EXT FRAC          RAF RATE          EXT RATE
   1       0.0573786        0.9385054             2.981           669.015
   2       0.9240133        0.0591209            48.012            42.144
   3       0.0186081        0.0023721             0.967             1.691
 TOT       0.9999999        0.9999983            51.960           712.851


STAGE NUMBER       12

COMP        RAF FRAC         EXT FRAC          RAF RATE          EXT RATE
   1       0.0572450        0.9392151             0.345           668.969
   2       0.9327525        0.0595101             5.625            42.387
   3       0.0100025        0.0012728             0.060             0.907
 TOT       1.0000000        0.9999979             6.030           712.264
```

```
ITERATION NUMBER    15

DESCRIPTION                  STAGE          RATE
RAFFINATE PRODUCT             12           6.040
EXTRACT PRODUCT                1         760.296

STAGE      RAF RATE        EXT RATE
  1        101.871         760.296
  2         94.266         762.168
  3         85.444         754.562
  4         76.463         745.739
  5         68.517         736.759
  6         62.350         728.813
  7         58.048         722.645
  8         55.271         718.343
  9         53.568         715.565
 10         52.558         713.863
 11         51.970         712.853
 12          6.040         712.264

STAGE NUMBER          1

COMP       RAF FRAC        EXT FRAC        RAF RATE        EXT RATE
  1       0.0628471       0.8759613          6.402         665.990
  2       0.2313376       0.0188949         23.567          14.366
  3       0.7058153       0.1051424         71.902          79.939
 TOT      0.9999999       0.9999985        101.871         760.296

STAGE NUMBER          2

COMP       RAF FRAC        EXT FRAC        RAF RATE        EXT RATE
  1       0.0624307       0.8822106          5.885         672.392
  2       0.2950344       0.0235281         27.812          17.932
  3       0.6425348       0.0942597         60.569          71.842
 TOT      0.9999999       0.9999985         94.266         762.168

STAGE NUMBER          3

COMP       RAF FRAC        EXT FRAC        RAF RATE        EXT RATE
  1       0.0618493       0.8904175          5.285         671.875
  2       0.3803622       0.0293911         32.500          22.177
  3       0.5577885       0.0801902         47.659          60.508
 TOT      0.9999999       0.9999988         85.444         754.562
```

```
STAGE NUMBER        4

COMP          RAF FRAC         EXT FRAC        RAF RATE        EXT RATE
   1         0.0611262        0.9001462           4.674         671.274
   2         0.4840831        0.0360250          37.014          26.865
   3         0.4547907        0.0638276          34.775          47.599
 TOT         0.9999999        0.9999988          76.463         745.739

STAGE NUMBER        5

COMP          RAF FRAC         EXT FRAC        RAF RATE        EXT RATE
   1         0.0603109        0.9102894           4.132         670.663
   2         0.5953858        0.0425921          40.794          31.380
   3         0.3443032        0.0471171          23.591          34.714
 TOT         0.9999999        0.9999985          68.517         736.759

STAGE NUMBER        6

COMP          RAF FRAC         EXT FRAC        RAF RATE        EXT RATE
   1         0.0594819        0.9194701           3.709         670.121
   2         0.6991132        0.0482427          43.590          35.160
   3         0.2414048        0.0322854          15.052          23.530
 TOT         0.9999999        0.9999982          62.350         728.813

STAGE NUMBER        7

COMP          RAF FRAC         EXT FRAC        RAF RATE        EXT RATE
   1         0.0587361        0.9267308           3.409         669.698
   2         0.7832955        0.0525229          45.468          37.955
   3         0.1579685        0.0207445           9.170          14.991
 TOT         1.0000000        0.9999981          58.048         722.645

STAGE NUMBER        8

COMP          RAF FRAC         EXT FRAC        RAF RATE        EXT RATE
   1         0.0581479        0.9318646           3.214         669.398
   2         0.8440309        0.0554530          46.650          39.834
   3         0.0978211        0.0126806           5.407           9.109
 TOT         0.9999999        0.9999982          55.271         718.343
```

```
STAGE NUMBER        9

COMP          RAF FRAC         EXT FRAC          RAF RATE          EXT RATE
   1         0.0577335        0.9352082             3.093           669.203
   2         0.8841447        0.0573194            47.362            41.016
   3         0.0581218        0.0074710             3.[illegible]13             5.346
 TOT         1.0000000        0.9999985            53.568           715.565

STAGE NUMBER       10

COMP          RAF FRAC         EXT FRAC          RAF RATE          EXT RATE
   1         0.0574641        0.9372682             3.020           669.081
   2         0.9090924        0.0584535            47.780            41.728
   3         0.0334436        0.0042765             1.758             3.053
 TOT         0.9999999        0.9999982            52.558           713.863

STAGE NUMBER       11

COMP          RAF FRAC         EXT FRAC          RAF RATE          EXT RATE
   1         0.0572984        0.9384946             2.978           669.008
   2         0.9240260        0.0591229            48.022            42.146
   3         0.0186757        0.0023807             0.971             1.697
 TOT         1.0000000        0.9999982            51.970           712.853

STAGE NUMBER       12

COMP          RAF FRAC         EXT FRAC          RAF RATE          EXT RATE
   1         0.0571992        0.9392099             0.346           668.966
   2         0.9327610        0.0595107             5.634            42.387
   3         0.0100398        0.0012775             0.061             0.910
 TOT         0.9999999        0.9999982             6.040           712.264
```

```
DESIGN TO SPECIFICATION CHECK



    SPECIFICATION TYPE        3
    CONTROL CODE              2

    SPECIFICATION VALUE            1.000000E-02
    CURRENT VALUE                  1.003983E-02

    PRESENT VALUE OF CONTROL                      666.334470
    COMPUTED CORRECTION TO CONTROL                  0.000000
    ESTIMATED VALUE OF CONTROL                    666.334470
    FINAL VALUE OF CONTROL                        666.334470
```

```
ITERATION NUMBER    16

DESCRIPTION                   STAGE          RATE
RAFFINATE PRODUCT              12           6.040
EXTRACT PRODUCT                 1         760.297

STAGE         RAF RATE        EXT RATE
   1           101.869         760.297
   2            94.265         762.166
   3            85.445         754.561
   4            76.462         745.741
   5            68.513         736.759
   6            62.343         728.809
   7            58.040         722.639
   8            55.264         718.335
   9            53.563         715.560
  10            52.555         713.858
  11            51.968         712.850
  12             6.040         712.263

STAGE NUMBER        1

COMP         RAF FRAC        EXT FRAC         RAF RATE        EXT RATE
   1        0.0628500       0.8759604            6.402         665.990
   2        0.2313369       0.0188954           23.566          14.366
   3        0.7058131       0.1051424           71.901          79.939
 TOT        0.9999999       0.9999982          101.869         760.297

STAGE NUMBER        2

COMP         RAF FRAC        EXT FRAC         RAF RATE        EXT RATE
   1        0.0624569       0.8822121            5.887         672.392
   2        0.2950237       0.0235280           27.810          17.932
   3        0.6425192       0.0942577           60.567          71.840
 TOT        0.9999999       0.9999978           94.265         762.166

STAGE NUMBER        3

COMP         RAF FRAC        EXT FRAC         RAF RATE        EXT RATE
   1        0.0618805       0.8904210            5.287         671.877
   2        0.3803469       0.0293898           32.499          22.176
   3        0.5577726       0.0801873           47.659          60.506
 TOT        1.0000000       0.9999982           85.445         754.561
```

```
STAGE NUMBER        4

COMP        RAF FRAC        EXT FRAC        RAF RATE      EXT RATE
   1       0.0611171       0.9001468          4.673        671.276
   2       0.4840922       0.0360242         37.015         26.865
   3       0.4547907       0.0638266         34.774         67.598
 TOT       1.0000000       0.9999976         76.462        765.741

STAGE NUMBER        5

COMP        RAF FRAC        EXT FRAC        RAF RATE      EXT RATE
   1       0.0602317       0.9102879          4.127        670.662
   2       0.5954543       0.0425931         40.796         31.381
   3       0.3443140       0.0471168         23.590         34.714
 TOT       0.9999999       0.9999977         68.513        736.759

STAGE NUMBER        6

COMP        RAF FRAC        EXT FRAC        RAF RATE      EXT RATE
   1       0.0593460       0.9194665          3.700        670.115
   2       0.6992445       0.0482466         43.593         35.163
   3       0.2414095       0.0322848         15.050         23.529
 TOT       1.0000000       0.9999978         62.343        728.809

STAGE NUMBER        7

COMP        RAF FRAC        EXT FRAC        RAF RATE      EXT RATE
   1       0.0585874       0.9267264          3.400        669.688
   2       0.7834517       0.0525286         45.471         37.959
   3       0.1579608       0.0207429          9.168         14.990
 TOT       0.9999999       0.9999978         58.040        722.639

STAGE NUMBER        8

COMP        RAF FRAC        EXT FRAC        RAF RATE      EXT RATE
   1       0.0580215       0.9318616          3.207        669.389
   2       0.8441719       0.0554580         46.652         39.837
   3       0.0978066       0.0126785          5.405          9.107
 TOT       0.9999999       0.9999980         55.264        718.335
```

```
STAGE NUMBER        9

COMP          RAF FRAC        EXT FRAC         RAF RATE        EXT RATE
   1         0.0576417       0.9352045            3.087         669.194
   2         0.8842506       0.0573238           47.363          41.019
   3         0.0581076       0.0074691            3.112           5.345
 TOT         0.9999999       0.9999974           53.563         715.560

STAGE NUMBER       10

COMP          RAF FRAC        EXT FRAC         RAF RATE        EXT RATE
   1         0.0574043       0.9372664            3.017         669.075
   2         0.9091629       0.0584563           47.781          41.729
   3         0.0334329       0.0042751            1.757           3.052
 TOT         0.9999999       0.9999977           52.555         713.858

STAGE NUMBER       11

COMP          RAF FRAC        EXT FRAC         RAF RATE        EXT RATE
   1         0.0572620       0.9384935            2.976         669.005
   2         0.9240694       0.0591244           48.022          42.147
   3         0.0186687       0.0023798            0.970           1.696
 TOT         1.0000000       0.9999977           51.968         712.850

STAGE NUMBER       12

COMP          RAF FRAC        EXT FRAC         RAF RATE        EXT RATE
   1         0.0571786       0.9392086            0.345         668.963
   2         0.9327856       0.0595122            5.634          42.388
   3         0.0100358       0.0012770            0.061           0.910
 TOT         0.9999999       0.9999977            6.040         712.263
```

```
FINAL MATERIAL BALANCE


INPUT SUMMARY


              COMP 1     COMP 2     COMP 3      TOTAL


FEED 1         0.000     20.000     80.000    100.000
FEED 2       666.333      0.000      0.000    666.334

TOTAL        666.333     20.000     80.000    766.333


OUTPUT SUMMARY


              COMP 1     COMP 2     COMP 3      TOTAL


RAF PROD       0.345      5.634      0.061      6.040
EXT PROD     665.990     14.366     79.939    760.297

TOTAL        666.335     20.000     80.000    766.335


**FORTRAN ** STOP

03RT  00:16:20
```

PROGRAM LISTING

```
      PROGRAM LIQLIQ
C
C     PROGRAM  "LIQLIQ"   :  LIQUID-LIQUID EXTRACTION PROGRAM USING
C                            THE FOUR SUFFIX MARGULES EQUATION FOR A
C                            TERNARY SYSTEM
C
C     MAIN CONTROL FOR PROGRAM  "LIQLIQ"
C
C     AUTHOR:   EDWARD C. ROCHE, JR.
C               NEWARK COLLEGE OF ENGINEERING
C               323 HIGH STREET
C               NEWARK, NEW JERSEY   07102
C
C     MAIN PROGRAM
C
      COMMON   /LIQEXT/  B(20,20), A(20,20), C(20,20,29), D(20,30,5),
     1                   XL(30), XV(30), X(9,30), Y(9,30), FD(7),
     2                   FX(9,8), IFX(7), R(5), IR(5), E(5), IE(5),
     3                   XRR, REC(9), KXR, NSTAGE, NCOMP, RMAX,
     4                   FTEST, STEST, NSPEC, NRHS, ISPEC(4), ISTAGE(4),
     5                   ICOMP(4), SPEC(4), JCTRL(4), NPRNT, MAX. NTIME,
     6                   K1, K2, K3, NL, NV, NPUNCH
C
      REAL               PAGE(2), RX(9), EY(9)
      EQUIVALENCE        (RX,B), (EY,A)
      DIMENSION          NT(20,3)
      EQUIVALENCE        (B(1,1),NT(1,1))
C
      DATA     PAGE   /  8H(1H1)      /
C
C     INPUT INFORMATION IS READ FROM CARD READER   --  K1=5
C     OUTPUT INFORMATION IS WRITTEN ON PRINTER     --  K2=6
C     FINAL INTERNAL FLOW RATES AND COMPOSITIONS
C         ARE PUNCHED BY CARD PUNCH                --  K3=7
C
      K1 = 5
      K2 = 6
      K3 = 7
C
C     TITLE CARDS
  999 DO  1    J=1,3
    1 READ (K1,2,END=9999) (NT(I,J),I=1,20)
    2 FORMAT (20A4)
C
      WRITE ( K2, PAGE )
      WRITE ( K2, PAGE )
      WRITE ( K2, 8 )
    8 FORMAT (////)
      DO  4    N=1,3
    4 WRITE (K2,5) (NT(I,N),I=1,20)
    5 FORMAT (T5,20A4)
C
C     CLEAR COMMON /LIQEXT/ FROM XL(1) TO NTIME
      CALL CLEAR ( XL, 747 )
C
      CALL IO ( 1 )
C
C         MAX        MAXIMUM NUMBER OF ITERATIONS
C         NFIX       ITERATION COUNTER
C         NDONE      CONVERGENCE CONTROL  (0=YES 1=NO)
C
      IF ( MAX .LE. 0 ) MAX=20
   69 NFIX = 0
      NDONE = 0
C
C     INTERMEDIATE PRINT-OUT CONTROL IS BY "NPRNT"
C
C         X          RAFFINATE COMPOSITIONS
C         Y          EXTRACT COMPOSITIONS
C         RX         RAFFINATE COMPONENTIAL RATE
C         EY         EXTRACT COMPONENTIAL RATE
C         XL         TOTAL RAFFINATE FLOW RATE
C         XV         TOTAL EXTRACT FLOW RATE
C
   70 IF ( NDONE .GT. 0 ) GO TO 71
      IF ( NPRNT .LT. 2 ) GO TO 86
   71 WRITE ( K2, 72 ) NFIX
   72 FORMAT (17H1ITERATION NUMBERI5//12H0DESCRIPTION,13X,5HSTAGE,11X,4H
     1RATE)
      WRITE ( K2, 73 )
   73 FORMAT (18H RAFFINATE PRODUCT)
      WRITE ( K2, 74 ) NSTAGE, XL(NSTAGE)
   74 FORMAT (1H+,24X,I5,F15.3)
      IF ( KXR .EQ. 0 ) GO TO 77
      N = 1
      SUM = XL(N) / XRR
      WRITE ( K2, 75 )
   75 FORMAT (16H EXTRACT PRODUCT)
      WRITE ( K2, 74 ) N, SUM
      WRITE ( K2, 76 )
   76 FORMAT (18H RECOVERED SOLVENT)
      WRITE ( K2, 74 ) N, XV(N)
      GO TO 79
   77 N = 1
      WRITE ( K2, 75 )
      WRITE ( K2, 74 ) N, XV(N)
   79 WRITE ( K2, 80 ) (J,XL(J),XV(J),J=1,NSTAGE)
   80 FORMAT (//35H STAGE      RAF RATE       EXT RATE/(I5,2F15.3))
C
      IF ( NDONE .EQ. 1 ) GO TO 81
      IF ( NPRNT .LT. 3 ) GO TO 86
   81 LINE = 8 + NSTAGE
      IF ( KXR .NE. 0 ) LINE = LINE + 1
      NN = 6 + NCOMP
      DO  85    I=1,NSTAGE
      SR = 0.0
      SE = 0.0
      DO  82    J=1,NCOMP
      RX(J) = XL(I)*X(J,I)
      EY(J) = XV(I)*Y(J,I)
      SR = SR + X(J,I)
      SE = SE + Y(J,I)
   82 CONTINUE
      IF ( LINE+NN .GT. 50 ) LINE = 0
      IF ( LINE .EQ. 0 ) WRITE ( K2, PAGE )
      WRITE ( K2, 83 ) I, (J,X(J,I),Y(J,I),RX(J),EY(J),J=1,NCOMP)
   83 FORMAT (/13HOSTAGE NUMBERI8/5HOCOMP, 7X,8HRAF FRAC, 7X,8HEXT FRAC,
     1 7X,8HRAF RATE, 7X, 8HEXT RATE/(I5,2F15.7,2F15.3))
      WRITE ( K2, 84 ) SR, SE, XL(I), XV(I)
   84 FORMAT (5H  TOT,2F15.7,2F15.3)
      LINE = LINE + NN
   85 CONTINUE
      IF ( NDONE .GT. 0 ) GO TO 130
C
C     NORMALIZE COMPOSITIONS
C
   86 DO  89    N=1,NSTAGE
      SR = 0.0
      SE = 0.0
      DO  87    J=1,NCOMP
      SR = SR + X(J,N)
      SE = SE + Y(J,N)
   87 CONTINUE
      DO  88    J=1,NCOMP
      X(J,N) = X(J,N) / SR
      Y(J,N) = Y(J,N) / SE
   88 CONTINUE
   89 CONTINUE
C
C     LINEARIZE ALL EQUATIONS AND COMPUTE CORRECTIONS
C
      CALL MATRIX
C
C     LIMIT SIZE OF CORRECTIONS TO COMPOSITIONS
C
C        D(*,*,1) CONTAINS CORRECTIONS TO X, Y, XL, & XV FOR EACH STAGE
   90 DO  96    N=1,NSTAGE
      DO  95    LV=1,2
      DO  94    J=1,NCOMP
      GO TO ( 91, 92 ), LV
   91 XY = X(J,N) + D(J,N,1)
      GO TO 93
   92 L = J + NCOMP
      XY = Y(J,N) + D(L,N,1)
   93 IF ( XY .LT. 0.0  .OR.  XY .GT. 1.0 ) GO TO 100
   94 CONTINUE
   95 CONTINUE
   96 CONTINUE
      GO TO 105
C
  100 NN = 2*NCOMP
      DO  102  N=1,NSTAGE
      DO  101  K=1,NN
      D(K,N,1) = D(K,N,1)/2.0
  101 CONTINUE
  102 CONTINUE
      GO TO 90
C
C     LIMIT SIZE OF CORRECTIONS TO NET FLOW RATES
C
  105 DO  108  N=1,NSTAGE
      XY = AMIN1 ( ABS(D(NL,N,1)), RMAX*XL(N) )
      D(NL,N,1) = SIGN ( XY, D(NL,N,1) )
      XY = AMIN1 ( ABS(D(NV,N,1)), RMAX*XV(N) )
      D(NV,N,1) = SIGN ( XY, D(NV,N,1) )
  108 CONTINUE
C
C     CONVERGENCE CHECK
C
  110 SUM = 0.0
      SR  = 0.0
      SE  = 0.0
      DO  112  N=1,NSTAGE
      DO  111  J=1,NCOMP
      SR = AMAX1 ( ABS(D(J,N,1))/X(J,N), SR )
      L = J + NCOMP
      SE = AMAX1 ( ABS(D(L,N,1))/Y(J,N), SE )
  111 CONTINUE
      SUM = AMAX1 ( ABS(D(NL,N,1))/XL(N), ABS(D(NV,N,1))/XV(N), SUM )
  112 CONTINUE
  114 IF ( SR .LT. FTEST  .AND.  SE .LT. FTEST  .AND.
     1    SUM .LT. STEST ) NDONE = 1
C
      IF ( NSPEC .EQ. 0 ) GO TO 120
      IF ( NDONE .NE. 0 ) CALL CHECK ( NCHECK)
      IF ( NCHECK .EQ. 0 )  NDONE = 0
C
C     MAKE NECESSARY ADJUSTMENTS AND CHECK ITERATION COUNTER
C
  120 DO  123  N=1,NSTAGE
```

```
      DO  122  J=1,NCOMP
      X(J,N) = X(J,N) + D(J,N,1)
      L = J + NCOMP
      Y(J,N) = Y(J,N) + D(L,N,1)
  122 CONTINUE
      XL(N) = XL(N) + D(NL,N,1)
      XV(N) = XV(N) + D(NV,N,1)
  123 CONTINUE
  126 NFIX = NFIX + 1
      IF ( NFIX .GT. MAX ) NDONE = 1
      GO TO 70
C
  130 CALL ID ( 2 )
      IF ( NPUNCH .NE. 0 ) CALL PUNCH
C
      GO TO 999
 9999 STOP
      END
```

```
          SUBROUTINE    IO ( IOIO )
C
C         SUBROUTINE  "IO"  HANDLES THE BULK OF THE PROGRAM INPUT/OUTPUT
C         ARGUMENT VALUES:  1 INPUT - TRANSFER TO #4
C                           2 OUTPUT - TRANSFER TO #130
C
          COMMON   /LIQEXT/  B(20,20), A(20,20), C(20,20,29), D(20,30,5),
         1                   XL(30), XV(30), X(9,30), Y(9,30), FD(7),
         2                   FX(9,8), IFX(7), R(5), IR(5), E(5), IE(5),
         3                   XRR, REC(9), KXR, NSTAGE, NCOMP, RMAX,
         4                   FTEST, STEST, NSPEC, NRHS, ISPEC(4), ISTAGE(4),
         5                   ICOMP(4), SPEC(4), JCTRL(4), NPRNT, MAX, NTIME,
         6                   K1, K2, K3, NL, NV, NPUNCH
C
          DIMENSION          DEL(9,2), RX(9), EY(9), W(9), Z(9),
         1                   AFOR(7), BFOR(2,10),
         2                   JFOR(4), KFOR(6), LFOR(7), MFOR(5), NFOR(6),
         3                   JKLMN(10), SPACE(1)
          EQUIVALENCE        (DEL,A), (RX,A), (EY,B), (W,C), (Z,D)
C
C
          DATA     AFOR   /  28HFD 1FD 2FD 3FD 4FD 5FD 6FD 7  /
          DATA     BFOR   /  80HCOMP 1  COMP 2  COMP 3  COMP 4  COMP 5  COMP
         1 6  COMP 7  COMP 8  COMP 9   TOTAL     /
          DATA     JFOR   /  16H(I5,     F15.3)    /
          DATA     KFOR   /  24H(5H  TOT,        F15.3)    /
          DATA     LFOR   /  28H(5H FEED,I2,3X,      F10.3)    /
          DATA     MFOR   /  20H(1H+,9X,     F10.3)    /
          DATA     NFOR   /  24H(1H+,I8,1X,      F10.3)    /
          DATA     JKLMN  /  40H    1    2    3    4    5    6    7    8    9   10  /
          DATA     SPACE  /  4H(/)   /
C
C
          GO TO ( 4, 130 ), IOIO
C
C         READ CONTROL CODES
C              NSTAGE          TOTAL NUMBER OF STAGES
C              NCOMP           NUMBER OF COMPONENTS
C              KXR             CODE FOR EXTRACT REFLUX              0=NO  1=YES
C              NFD             NUMBER OF FEED STREAMS
C              NRP             NUMBER OF SIDE-PRODUCT STREAMS ( RAFFINATE )
C              NEP             NUMBER OF SIDE-PRODUCT STREAMS ( EXTRACT   )
C              NLV             STREAM RATES                         0=NO  1=YES
C              NXY             STREAM COMPOSITIONS                  0=NO  1=YES
C              MAX             MAXIMUM NUMBER OF ITERATIONS
C              NPRNT           OUTPUT CODE
C                                         1   INPUT PLUS CONVERGED CASE
C                                         2   1 PLUS SUMMARY OF ALL ITERATIONS
C                                         3   2 PLUS COMPOSITIONS AND RATES
C                                         4   3 PLUS ERRORS AND CORRECTIONS
```

```
C         NSPEC           NUMBER OF DESIGN SPECIFICATIONS
C         NPUNCH          PUNCH OPTION   0=NO  1=YES
C
    4 READ ( K1, 5 ) NSTAGE, NCOMP, KXR, NFD, NRP, NEP, NLV, N,Y,
     1                MAX, NPRNT, NSPEC, NPUNCH
    5 FORMAT (12I4)
      IF ( NPRNT .LE. 0  .OR.  NPRNT .GE. 5 ) NPRNT=1
C
      WRITE ( K2, 7 ) NSTAGE, NCOMP, KXR, NSPEC
    7 FORMAT (///23H0TOTAL NUMBER OF STAGESI5/21H NUMBER OF COMPONENTSI7
     1/20H EXTRACT REFLUX CODEI8/25H NUMBER OF SPECIFICATIONSI3)
C
C     TOLERANCES FOR CONVERGENCE TEST
C               FTEST     DELTA X / X  AND  DELTA Y / Y
C               STEST     DELTA XL / XL  AND  DELTA XV / XV
C               RMAX      DELTA FLOW / FLOW LIMITATION PER ITERATION
C
      READ ( K1, 12 ) FTEST, STEST, RMAX
      IF ( RMAX .LE. 0.0 ) RMAX = 0.50
      WRITE ( K2, 9 ) FTEST, STEST, RMAX
    9 FORMAT (///33H0TOLERANCES ON COMPUTED VARIABLES/5X12HCOMPOSITIONS
     1F9.6/5X10HFLOW RATES F11.6 ///54H MAXIMUM FRACTIONAL CHANGE IN FLO
     2W RATES PER ITERATION F11.6)
C
C     SET CONTROLS FOR NEWTON RAPHSON CALCULATION
C
      NL = 2*NCOMP + 1
      NV = NL + 1
      NRHS = NSPEC + 1
C
C     READ INPUT STREAMS
C
      READ ( K1, 5 ) (IFX(K),K=1,NFD)
      DO  13    K=1,NFD
      READ ( K1, 12 ) (FX(J,K),J=1,NCOMP)
   12 FORMAT (9F8.4)
   13 CONTINUE
C
C     COMPUTE TOTAL COLUMN FEED & FEED NUMBER THAT CONTAINS THE PRIME
C     SOLVENT
C
      NSOL = 0
      FDD = 0.0
      DO  17    K=1,NFD
      FD(K) = 0.0
      DO  14    J=1,NCOMP
      FD(K) = FD(K) + FX(J,K)
   14 CONTINUE
      FDD = FDD + FD(K)
      IF ( IFX(K) .NE. NSTAGE ) GO TO 17
      NSOL = K
   17 CONTINUE
      JFOR(2) = JKLMN(NFD)
      KFOR(4) = JFOR(2)
      WRITE ( K2, 19 ) NFD, NSOL, (J,IFX(J),J=1,NFD)
   19 FORMAT (///23H0NUMBER OF FEED STREAMSI5/16H SOLVENT FEED IS,8X,I4/
     1/15H FEED      STAGE/(I5,I10))
      WRITE ( K2, 20 ) (AFOR(J),J=1,NFD)
   20 FORMAT (5H0COMP,7(11X,A4))
      WRITE ( K2, JFOR ) (J,(FX(J,K),K=1,NFD),J=1,NCOMP)
      WRITE ( K2, KFOR ) (FD(K),K=1,NFD)
C
C     READ SIDE-PRODUCT STREAMS ( RAFFINATE )
C
      IF ( NRP .EQ. 0 ) GO TO 26
      READ ( K1, 5 ) (IR(K),K=1,5)
      READ ( K1, 12 ) (R(K),K=1,5)
      WRITE ( K2, 21 ) NRP
   21 FORMAT (///40H0NUMBER OF RAFFINATE PRODUCT SIDESTREAMSI5)
      WRITE ( K2, 22 ) (IR(K),R(K),K=1,NRP)
   22 FORMAT (6H0STAGE,10X,4HRATE/(I5,F15.3))
C
C     READ SIDE-PRODUCT STREAMS ( EXTRACT )
C
   26 IF ( NEP .EQ. 0 ) GO TO 31
      READ ( K1, 5 ) (IE(K),K=1,5)
      READ ( K1, 12 ) (E(K),K=1,5)
      WRITE ( K2, 27 ) NEP
   27 FORMAT (///38H0NUMBER OF EXTRACT PRODUCT SIDESTREAMSI5)
      WRITE ( K2, 22 ) (IE(K),E(K),K=1,NEP)
C
C     DATA FOR SOLVENT RECOVERY SYSTEM
C
   31 IF ( KXR .EQ. 0 ) GO TO 37
      READ ( K1, 12 ) XRR
      READ ( K1, 12 ) (REC(J),J=1,NCOMP)
      DO  33   J=1,NCOMP
      IF ( REC(J) .GE. 1.0 ) REC(J) = 0.999999
      IF ( REC(J) .LE. 0.0 ) REC(J) = 0.000001
   33 CONTINUE
      WRITE ( K2, 35 ) XRR, (K,REC(K),K=1,NCOMP)
   35 FORMAT (///30H0EXTERNAL EXTRACT REFLUX RATIOF15.8////38H RECOVERIE
     1S IN SOLVENT RECOVERY SYSTEM/5H0COMP,7X,8HREC FRAC/(I5,F15.7))
C
C     READ IN KNOWN STREAM RATES
C
   37 IF ( NLV .EQ. 0 ) GO TO 38
      READ ( K1, 12 ) (XL(K),K=1,NSTAGE)
      READ ( K1, 12 ) (XV(K),K=1,NSTAGE)
      GO TO 60
```

```
C
C     ESTIMATE INTERNAL FLOW RATES BASED ON FEEDS AND SIDESTREAM WITHDRA
C
   38 DO  59   LV=1,2
      DO  58   I=1,NSTAGE
      GO TO ( 40, 39 ), LV
C     FOR RAFFINATE PHASE START AT THE TOP AND CALCULATE DOWN THE TOWER
   39 N = I
      GO TO 42
C     FOR EXTRACT PHASE START AT THE BOTTOM AND CALCULATE UP THE TOWER
   40 N = NSTAGE + 1 - I
   42 RR  = 0.0
      EE  = 0.0
      FFX = 0.0
      DO  46  K=1,7
      IF ( K .GT. 5 ) GO TO 44
      IF ( N .NE. IR(K) ) GO TO 43
      RR = R(K)
   43 IF ( N .NE. IE(K) ) GO TO 44
      EE = E(K)
   44 IF ( N .NE. IFX(K) ) GO TO 46
      FFX = FD(K)
   46 CONTINUE
      GO TO ( 53, 47 ), LV
   47 IF ( N .GT. 1 ) GO TO 51
      IF ( KXR .NE. 0 ) GO TO 49
      XL(N) = XV(N+1) + FFX - XV(N) - RR
      GO TO 58
   49 XL(N) = ( FDD - FD(NSOL) ) / 2.0 * XRR
      GO TO 58
   51 IF ( N .EQ. NSTAGE ) GO TO 52
      XL(N) = XL(N-1) + XV(N+1) + FFX - XV(N) - RR - EE
      GO TO 58
   52 XL(N) = XL(N-1) + FFX - XV(N) - EE
      GO TO 58
   53 IF ( N .GT. 1 ) GO TO 55
      IF ( KXR .NE. 0 ) GO TO 54
      XV(N) = XV(N+1)
      GO TO 58
   54 XV(N) = FD(NSOL)
      GO TO 58
   55 IF ( N .EQ. NSTAGE ) GO TO 56
      XV(N) = XV(N+1) + 0.5*FFX - EE
      GO TO 58
   56 XV(N) = FFX - EE
   58 CONTINUE
   59 CONTINUE
C
C     READ IN COMPOSITION DATA
C
```

```
   60 IF ( NXY .EQ. 0 ) GO TO 65
      DO  62   K=1,NSTAGE
      READ ( K1, 12 ) (X(J,K),J=1,NCOMP)
      DO  61   J=1,NCOMP
      IF ( X(J,K) .LE. 0.0 ) X(J,K) = 0.000001
      IF ( X(J,K) .GE. 1.0 ) X(J,K) = 0.999999
   61 CONTINUE
   62 CONTINUE
      DO  64   K=1,NSTAGE
      READ ( K1, 12 ) (Y(J,K),J=1,NCOMP)
      DO  63   J=1,NCOMP
      IF ( Y(J,K) .LE. 0.0 ) Y(J,K) = 0.000001
      IF ( Y(J,K) .GE. 1.0 ) Y(J,K) = 0.999999
   63 CONTINUE
   64 CONTINUE
      GO TO 69
C
C     READ ESTIMATED COMPOSITIONS FOR STAGE  1  AND  NSTAGE
C     AND FROM THESE ESTIMATE THE REMAINING COMPOSITIONS
C
   65 READ ( K1, 12 ) (X(J,1),J=1,NCOMP)
      READ ( K1, 12 ) (X(J,NSTAGE),J=1,NCOMP)
      READ ( K1, 12 ) (Y(J,1),J=1,NCOMP)
      READ ( K1, 12 ) (Y(J,NSTAGE),J=1,NCOMP)
      NN = NSTAGE -1
      XY = FLOAT( NN )
      DO  66   J=1,NCOMP
      IF ( X(J,1) .LE. 0.0 ) X(J,1) = 0.000001
      IF ( Y(J,1) .LE. 0.0 ) Y(J,1) = 0.000001
      IF ( X(J,1) .GE. 1.0 ) X(J,1) = 0.999999
      IF ( Y(J,1) .GE. 1.0 ) Y(J,1) = 0.999999
      IF ( X(J,NSTAGE) .LE. 0.0 ) X(J,NSTAGE) = 0.000001
      IF ( Y(J,NSTAGE) .LE. 0.0 ) Y(J,NSTAGE) = 0.000001
      IF ( X(J,NSTAGE) .GE. 1.0 ) X(J,NSTAGE) = 0.999999
      IF ( Y(J,NSTAGE) .GE. 1.0 ) Y(J,NSTAGE) = 0.999999
      DEL(J,1) = (X(J,1)-X(J,NSTAGE)) / XY
      DEL(J,2) = (Y(J,1)-Y(J,NSTAGE)) / XY
   66 CONTINUE
      DO  68   K=2,NN
      DO  67   J=1,NCOMP
      X(J,K) = X(J,K-1) - DEL(J,1)
      Y(J,K) = Y(J,K-1) - DEL(J,2)
   67 CONTINUE
   68 CONTINUE
C
C     READ IN SPECIFICATION INFORMATION
C
C     DESIGN SPECIFICATION INFORMATION
C        ISPEC          CODE FOR TYPE OF SPECIFICATION
C                         1    RAFFINATE RATE  (XL)
```

```
C                          2    EXTRACT RATE      (XV)
C                          3    RAFFINATE COMPOSITION  (X)
C                          4    EXTRACT COMPOSITION    (Y)
C         ISTAGE       STAGE SPECIFICATION IS ON
C         ICOMP        COMPONENT COMPOSITION SPECIFICATION IS ON
C         SPEC         VALUE OF SPECIFICATION
C         JCTRL        CONTROL PARAMETER
C                          1    FEED STREAM NUMBER 1
C                          2    FEED STREAM NUMBER 2
C                          ETC
C
   69 IF ( NSPEC .EQ. 0 ) GO TO 999
      READ ( K1, 71 ) (ISPEC(J),ISTAGE(J),ICOMP(J),SPEC(J),JCTRL(J),
     1               J=1,NSPEC)
   71 FORMAT (3I8,F8.4,I8)
      WRITE ( K2, 73 ) (J,ISPEC(J),ISTAGE(J),ICOMP(J),SPEC(J),JCTRL(J),
     1                 J=1,NSPEC)
   73 FORMAT (///29H0DESIGN SPECIFICATION OPTIONS/46H0NO  TYPE  STAGE  C
     1OMP NO  SPEC VALUE  CONTROL/(I3,I6,2I7,1PE14.4,I6))
      GO TO 999
C
C     ******************************************************************
C
C     MATERIAL BALANCE SUMMARY
C
  130 WRITE ( K2, 131 )
  131 FORMAT (23H1FINAL MATERIAL BALANCE///14H0INPUT SUMMARY//)
      WRITE ( K2, 132 ) ((BFOR(N,J),N=1,2),J=1,NCOMP),
     1                   (BFOR(N,10),N=1,2)
  132 FORMAT (10X,10(2X,2A4))
      WRITE ( K2, SPACE )
      LFOR(5) = JKLMN(NCOMP+1)
  136 WRITE ( K2, LFOR ) (K,(FX(J,K),J=1,NCOMP),FD(K),K=1,NFD)
      XY = 0.0
      DO  138  J=1,NCOMP
      W(J) = 0.0
      DO  137  K=1,NFD
      W(J) = W(J) + FX(J,K)
  137 CONTINUE
      XY = XY + W(J)
  138 CONTINUE
      WRITE ( K2, 139 )
  139 FORMAT (6H0TOTAL)
      MFOR(3) = JKLMN(NCOMP+1)
      WRITE ( K2, MFOR ) (W(J),J=1,NCOMP), XY
C
  140 WRITE ( K2, 141 )
  141 FORMAT (//15H0OUTPUT SUMMARY//)
      WRITE ( K2, 132 ) ((BFOR(N,J),N=1,2),J=1,NCOMP),
     1                   (BFOR(N,10),N=1,2)
```

```
          WRITE ( K2, SPACE )
          DO  142  J=1,NCOMP
          Z(J) = 0.0
     142  CONTINUE
          IF ( KXR .NE. 0 ) GO TO 160
          DO  152  J=1,NCOMP
          RX(J) = XL(NSTAGE) * X(J,NSTAGE)
          EY(J) = XV(1) * Y(J,1)
          Z(J) = RX(J) + EY(J)
     152  CONTINUE
          WRITE ( K2, 154 )
     154  FORMAT (9H RAF PROD)
          WRITE ( K2, MFOR ) (RX(J),J=1,NCOMP), XL(NSTAGE)
          WRITE ( K2, 155 )
     155  FORMAT (9H EXT PROD)
          WRITE ( K2, MFOR ) (EY(J),J=1,NCOMP), XV(1)
          GO TU 170
     160  WW = XL(1) / XRR
          DO  161  J=1,NCOMP
          RX(J) = XL(NSTAGE) * X(J,NSTAGE)
          W(J) = WW * X(J,1)
          EY(J) = XV(1) * Y(J,1)
          Z(J) = RX(J) + W(J) + EY(J)
     161  CONTINUE
          WRITE ( K2, 154 )
          WRITE ( K2, MFOR ) (RX(J),J=1,NCOMP), XL(NSTAGE)
          WRITE ( K2, 155 )
          WRITE ( K2, MFOR ) (W(J),J=1,NCOMP), WW
          WRITE (K2, 164 )
     164  FORMAT (9H REC SOLV)
          WRITE ( K2, MFOR ) (EY(J),J=1,NCOMP), XV(1)
     170  NFOR(4) = MFOR(3)
          IF ( NRP .EQ. 0 ) GO TO 180
          DO  175  N=1,NRP
          K = IR(N)
          DO  172  J=1,NCOMP
          RX(J) = R(N) * X(J,K)
          Z(J) = Z(J) + RX(J)
     172  CONTINUE
          WRITE ( K2, 173 )
     173  FORMAT (7H RAF SS)
          WRITE ( K2, NFOR ) N, (RX(J),J=1,NCOMP), R(N)
     175  CONTINUE
     180  IF ( NEP .EQ. 0 ) GO TO 190
          DO  185  N=1,NEP
          K = IE(N)
          DO  182  J=1,NCOMP
          EY(J) = E(N) * Y(J,K)
          Z(J) = Z(J) + EY(J)
     182  CONTINUE
```

```
      WRITE ( K2, 183 )
  183 FORMAT (7H EXT SS)
      WRITE ( K2, NFOR ) N, (EY(J),J=1,NCOMP), E(N)
  185 CONTINUE
  190 XY = 0.0
      DO  191  J=1,NCOMP
      XY = XY + Z(J)
  191 CONTINUE
      WRITE ( K2, 139 )
      WRITE ( K2, MFOR ) (Z(J),J=1,NCOMP), XY
C
  999 RETURN
      END
      SUBROUTINE    MATRIX
C
C     SUBROUTINE "MATRIX"
C     EDITURIAL PROGRAM FOR THE SOLUTION OF THE TRIDIAGONAL MATRIX
C     REPRESENTING THE LINEARIZED LIQUID-LIQUID EXTRACTION
C     PROBLEM
C
C     NUMBER OF RIGHT HAND SIDES (RHS) EQUALS ONE MORE THAN THE
C     NUMBER OF DESIGN SPECIFICATIONS
C
      COMMON   /LIQEXT/  B(20,20), A(20,20), C(20,20,29), D(20,30,5),
     1                   XL(30), XV(30), X(9,30), Y(9,30), FD(7),
     2                   FX(9,8), IFX(7), R(5), IR(5), E(5), IE(5),
     3                   XRR, REC(9), KXR, NSTAGE, NCOMP, RMAX,
     4                   FTEST, STEST, NSPEC, NRHS, ISPEC(4), ISTAGE(4),
     5                   ICOMP(4), SPEC(4), JCTRL(4), NPRNT, MAX, NTIME,
     6                   K1, K2, K3, NL, NV, NPUNCH
C
      REAL               W(20)
      EQUIVALENCE        (W,A)
C
C
C     STAGE    1  THROUGH  NSTAGE
C
   40 DO  90    I=1,NSTAGE
C
C     GENERATE A, B, C, AND D
C
      CALL ABCD ( I )
C
C     CLEAR A AND ADJUST B AND D -- NEED ONLY
C        PERFORM ADJUSTMENT OF B AND D
C
      IF ( I .EQ. 1 ) GO TO 60
   50 DO  53    L=1,NV
      DO  52    K=1,NV
      O = 0.0
      DO  51    M=1,NV
      O = O + A(K,M)*C(M,L,I-1)
   51 CONTINUE
      B(K,L) = B(K,L) - O
   52 CONTINUE
   53 CONTINUE
      DO  56    J=1,NRHS
      DO  55    L=1,NV
      P = 0.0
      DO  54    K=1,NV
      P = P + A(L,K)*D(K,I-1,J)
   54 CONTINUE
      D(L,I,J) = D(L,I,J) - P
   55 CONTINUE
   56 CONTINUE
C
C     INVERT MATRIX B AND ADJUST C AND D
C
   60 CALL SPINV ( B, NV, 20 )
C
C     MULTIPLY THROUGH BY INVERSE -- NEED ONLY DO C AND D
C
      IF (I .EQ. NSTAGE ) GO TO 80
   70 DO  73    L=1,NV
      DO  72    K=1,NV
      A(K,L) = 0.0
      DO  71    M=1,NV
      A(K,L) = A(K,L) + B(K,M)*C(M,L,I)
   71 CONTINUE
   72 CONTINUE
   73 CONTINUE
      DO  75    L=1,NV
      DO  74    K=1,NV
      C(K,L,I) = A(K,L)
   74 CONTINUE
   75 CONTINUE
   80 DO  84    J=1,NRHS
      DO  82    K=1,NV
      W(K) = 0.0
      DO  81    M=1,NV
      W(K) = W(K) + B(K,M)*D(M,I,J)
   81 CONTINUE
   82 CONTINUE
      DO  83    K=1,NV
      D(K,I,J) = W(K)
   83 CONTINUE
   84 CONTINUE
   90 CONTINUE
C
C     CLEAR C BY BACK SUBSTITUTION -- WHEN FINISHED LHS
C         WILL BE IDENTITY MATRIX AND RHS WILL CONTAIN
C         DESIRED CORRECTIONS TO FLOW RATES AND COMPOSITIONS
C
C     STAGE    1  THROUGH  NSTAGE-1
C
      N = NSTAGE-1
      DO  95    NN=1,N
      I = N - NN + 1
      DO  94    J=1,NRHS
      DO  93    K=1,NV
      P = 0.0
      DO  92    M=1,NV
      P = P + C(K,M,I)*D(M,I+1,J)
   92 CONTINUE
      D(K,I,J) = D(K,I,J) - P
   93 CONTINUE
   94 CONTINUE
   95 CONTINUE
C
      IF ( NPRNT .NE. 4 ) GO TO 99
      WRITE ( K2, 96 )
   96 FORMAT (21H1COMPUTED CORRECTIONS)
      DO  98   I=1,NSTAGE
      WRITE ( K2, 97 ) I, (D(M,I,1),M=1,NV)
   97 FORMAT (/I3,1P5E20.7/(3X,1P5E20.7))
   98 CONTINUE
C
   99 RETURN
      END
      SUBROUTINE    ABCD ( II )
C
C     SUBROUTINE "ABCD" GENERATES FOR STAGE 'II=I' THE ENTRIES IN THE
C       JACOBIAN AND THE RHS
C
C         A          STAGE 'I-1'
C         B          STAGE 'I'
C         C          STAGE 'I+1'
C         D          RHS
C
      COMMON   /LIQEXT/  B(20,20), A(20,20), C(20,20,29), D(20,30,5),
     1                   XL(30), XV(30), X(9,30), Y(9,30), FD(7),
     2                   FX(9,8), IFX(7), R(5), IR(5), E(5), IE(5),
     3                   XRR, REC(9), KXR, NSTAGE, NCOMP, RMAX,
     4                   FTEST, STEST, NSPEC, NRHS, ISPEC(4), ISTAGE(4),
     5                   ICOMP(4), SPEC(4), JCTRL(4), NPRNT, MAX, NTIME,
     6                   K1, K2, K3, NL, NV, NPUNCH
C
      COMMON   /EQDATA/  ACT(9,2), GAM(9,2), PGAM(9,9,2)
C
C
      I = II
      MCTRL = 0
      ZFAC = 0.0
      CALL CLEAR ( B, 800 )
C
      SUMX = 0.0
      DO  5    J=1,NCOMP
      SUMX = SUMX + X(J,I)
    5 CONTINUE
C
      IF ( I .GT. 1 ) GO TO 10
      IF ( NPRNT .NE. 4 ) GO TO 7
      WRITE ( K2, 6 )
    6 FORMAT (16H1COMPUTED ERRORS)
C
    7 CALL CLEAR ( C, 400*(NSTAGE-1) )
      CALL CLEAR ( D, 600*NRHS )
      IF ( KXR .GT. 0 ) GO TO 30
C
   10 RR = 0.0
      EE = 0.0
      FFX = 0.0
C
C     FEED STREAM #8 IS A ZERO STREAM NEEDED WHEN THE STAGE
C     HAS NO FEED
C
      IFFX = 8
      DO  14   K=1,7
      IF ( K .GT. 5 ) GO TO 12
      IF ( I .NE. IR(K) ) GO TO 11
      RR = R(K)
   11 IF ( I .NE. IE(K) ) GO TO 12
      EE = E(K)
   12 IF ( I .NE. IFX(K) ) GO TO 14
      IFFX = K
      FFX = FD(K)
   14 CONTINUE
      RL = RR + XL(I)
      EV = EE + XV(I)
C
      IF ( NSPEC .EQ. 0 ) GO TO 23
      IF ( IFFX .EQ. 8 ) GO TO 23
      DO  16   K=1,NSPEC
      IF ( JCTRL(K) .EQ. IFFX ) GO TO 17
   16 CONTINUE
      GO TO 23
   17 MCTRL = K + 1
C
   23 CALL ACTO ( I )
      DO  25   J=1,NCOMP
      DO  24   K=1,NCOMP
      KK = K + NCOMP
      B(J,K) = X(J,I) * PGAM(J,K,1)
      B(J,KK) = - Y(J,I) * PGAM(J,K,2)
   24 CONTINUE
      JJ = J + NCOMP
      B(J,J) = B(J,J) + GAM(J,1)
      B(J,JJ) = B(J,JJ) - GAM(J,2)
      D(J,I,1) = - ACT(J,1) + ACT(J,2)
      B(JJ,J) = - RL
      B(JJ,NL) = - X(J,I)
      B(JJ,JJ) = - EV
      B(JJ,NV) = - Y(J,I)
      D(JJ,I,1) = RL*X(J,I) + EV*Y(J,I) - FX(J,IFFX)
      B(NL,J) = 1.0
   25 CONTINUE
      D(NL,I,1) = 1.0 - SUMX
      B(NV,NL) = - 1.0
      B(NV,NV) = - 1.0
      D(NV,I,1) = RL + EV - FFX
C
      IF ( I .EQ. 1 ) GO TO 40
      IF ( I .EQ. NSTAGE ) GO TO 60
      GO TO 50
C
C     SPECIAL SET OF EQUATION TO HANDLE THE SOLVENT RECOVERY
C     SYSTEM ASSOCIATED WITH THE EXTRACT REFLUX
C
   30 FAC = (XRR+1.0) / XRR
```

```
      DO  31   J=1,NCOMP
      JJ = J + NCOMP
      B(J,JJ) = XV(1)
      B(J,NV) = Y(J,1)
      C(J,JJ,1) = - REC(J) * XV(2)
      C(J,NV,1) = - REC(J) * Y(J,2)
      D(J,1,1) = - XV(1)*Y(J,1) + REC(J)*XV(2)*Y(J,2)
      XY = 1.0 - REC(J)
      B(JJ,J) = XL(1) * FAC
      B(JJ,NL) = X(J,1) * FAC
      C(JJ,JJ,1) = - XV(2) * XY
      C(JJ,NV,1) = - Y(J,2) * XY
      D(JJ,1,1) = - XL(1)*X(J,1)*FAC + XV(2)*Y(J,2)*XY
      B(NL,J) = 1.0
   31 CONTINUE
      D(NL,1,1) = 1.0 - SUMX
      B(NV,NL) = FAC
      B(NV,NV) = 1.0
      C(NV,NV,1) = - 1.0
      D(NV,1,1) = - XL(1)*FAC - XV(1) + XV(2)
      GO TO 70
C
   40 DO  41   J=1,NCOMP
      JJ = J + NCOMP
      C(JJ,JJ,1) = XV(2)
      C(JJ,NV,1) = Y(J,2)
      D(JJ,1,1) = D(JJ,1,1) - XV(2)*Y(J,2)
   41 CONTINUE
      C(NV,NV,1) = 1.0
      D(NV,1,1) = D(NV,1,1) - XV(2)
      GO TO 70
C
   50 DO  51   J=1,NCOMP
      JJ = J + NCOMP
      A(JJ,J) = XL(I-1)
      A(JJ,NL) = X(J,I-1)
      C(JJ,JJ,I) = XV(I+1)
      C(JJ,NV,I) = Y(J,I+1)
      D(JJ,I,1) = D(JJ,I,1) - XL(I-1)*X(J,I-1) - XV(I+1)*Y(J,I+1)
   51 CONTINUE
      A(NV,NL) = 1.0
      C(NV,NV,I) = 1.0
      D(NV,I,1) = D(NV,I,1) - XL(I-1) - XV(I+1)
      GO TO 70
C
   60 DO  61   J=1,NCOMP
      JJ = J + NCOMP
      A(JJ,J) = XL(NSTAGE-1)
      A(JJ,NL) = X(J,NSTAGE-1)
      D(JJ,NSTAGE,1) = D(JJ,NSTAGE,1) - XL(NSTAGE-1)*X(J,NSTAGE-1)
   61 CONTINUE
      A(NV,NL) = 1.0
      D(NV,NSTAGE,1) = D(NV,NSTAGE,1) - XL(NSTAGE-1)
C
   70 IF ( NSPEC .EQ. 0 ) GO TO 90
      DO  72   N=2,NRHS
      DO  71   L=1,NV
      D(L,I,N) = D(L,I,1)
   71 CONTINUE
   72 CONTINUE
C
C     ..................................................................
C
C     INCREASE FFX BY 1.0
      IF ( MCTRL .EQ. 0 ) GO TO 90
      ZFAC = (FFX+1.0)/FFX - 1.0
      DO  74   J=1,NCOMP
      JJ = J + NCOMP
      D(JJ,I,MCTRL) = D(JJ,I,MCTRL) - FX(J,IFFX)*ZFAC
   74 CONTINUE
      D(NV,I,MCTRL) = D(NV,I,MCTRL) - 1.0
C
   90 IF ( NPRNT .NE. 4 ) GO TO 99
      WRITE ( K2, 91 ) I, (D(M,I,1),M=1,NV)
   91 FORMAT (/I3,1P5E20.7/(3X,1P5E20.7))
C
   99 RETURN
      END
      SUBROUTINE    SPINV ( A, M, KK )
C
C     SUBROUTINE "SPINV" IS A STANDARD SINGLE PRECISION MATRIX
C     INVERSION ROUTINE  ---  MATRIX GIVEN IN 'A(*,*)' AND INVERSE
C     DEVELOPED IN 'B(*,*)'. BEFORE RETURN INVERSE IS RELOADED INTO
C     'A(*,*)'.
C
C     DIMENSION A(KK,KK), B(KK,KK)
C     A  AND  B  ARE ASSUMED TO BE ADJACENT TO EACH OTHER
C
      DIMENSION A(1)
C
C
      ISIG = 0
      N = M
      NN = KK
      N2 = N + N
C
C     MAKE B THE IDENTITY MATRIX
C
      DO 11 J=1,N
      NJCOL = (N+J-1)*NN
      DO 10 I=1,N
      KINJ = NJCOL + I
      IF(I-J)4,6,4
    4 A(KINJ) = 0.
      GO TO 10
    6 A(KINJ) = 1.
   10 CONTINUE
   11 CONTINUE
C
C     DETERMINE MAX ABS OF VARIABLE BEING ELIMINATED  --  THIS BECOMES
C         PIVOTAL ROW
C
      L = 0
   12 L = L + 1
      LCOL = NN*L-NN
      KLL = LCOL + L
      IF(L - N)13,30,1000
C
C     FIND LARGEST ELEMENT IN LTH COLUMN
C
   13 J1 = L
      C = ABS ( A(KLL) )
      L1 = L + 1
      DO 20 I = L1,N
      KIL = LCOL + I
      X = ABS (A(KIL))
      IF(C - X)14,20,20
C
```

```
C     RECORD NUMBER OF ROW HAVING GREATER ELEMENT
C
   14 J1 = I
C
C     C BECOMES GREATER
C
      C  = X
   20 CONTINUE
C
C     INTERCHANGE ROW J1 WITH ROW L  --  J1 IS ROW WITH LARGEST ELEMENT
C     TEST TO SEE IF INTERCHANGE IS NECESSARY
C
      IF(J1 - L)22,30,22
   22 DO 24 J = L,N2
      JCOL = NN*J-NN
      KJIJ = JCOL + J1
      HOLD = A(KJIJ)
      KLJ = JCOL + L
      A(KJIJ) = A(KLJ)
      A(KLJ) = HOLD
   24 CONTINUE
C
C     IF LARGEST ABS VALUE OF ELEMENT IN A COLUMN IS ZERO  --  MATRIX
C          IS SINGULAR
C
   30 IF(ABS (A(KLL)) - .00000001)33,33,32
   33 WRITE (6,100)
  100 FORMAT(//20X,42H MATRIX IS SINGULAR, NO INVERSE OBTAINABLE///)
      STOP
C
C     ZERO ALL ELEMENTS IN LTH COLUMN EXCEPT PIVOTAL ELEMENT
C
   32 L1 = 1
      L2 = L - 1
      IF(L2)321,321,323
  321 IF(L-N)322,46,322
  322 L1 = L + 1
      L2 = N
  323 DO 324 I = L1,L2
      KIL = LCOL + I
      Z = -A(KIL)/A(KLL)
      DO 324 J = L,N2
      JCOL = NN*J - NN
      KIJ = JCOL + I
      KLJ = JCOL + L
      A(KIJ) = A(KIJ) + Z*A(KLJ)
  324 CONTINUE
      IF(N - L2)12,12,321
C
C     DIVIDE BY DIAGONAL ELEMENT
```

```
C
   46 DO 482 I=1,N
      KKK = NN*I - NN + I
      ZZ = A(KKK)
      DO 481 J=1,N2
      KKI = NN*J - NN + I
      A(KKI) = A(KKI)/ZZ
  481 CONTINUE
  482 CONTINUE
C
C     RETURN AFTER PUTTING A INVERSE INTO A FROM B
C
   49 DO 502 J=1,N
      JCOL = NN*J - NN
      NJCOL = NN * N + JCOL
      DO 501 I=1,N
      KIJ = JCOL + I
      KINJ = NJCOL + I
      A(KIJ) = A(KINJ)
  501 CONTINUE
  502 CONTINUE
C
 1000 RETURN
        END
      SUBROUTINE    CHECK ( NCHECK)
C
C     SUBROUTINE "CHECK" ASERTAINS IF THE DESIGN SPECIFICATIONS
C     HAVE BEEN SATISFIED.  IF SPECIFICATION HAS NOT BEEN SATISFIED
C     THEN CONTROL FEED STREAM TOTAL FLOW RATE IS ALTERED.
C
      COMMON   /LIQEXT/  B(20,20), A(20,20), C(20,20,29), D(20,30,5),
     1                   XL(30), XV(30), X(9,30), Y(9,30), FD(7),
     2                   FX(9,8), IFX(7), R(5), IR(5), E(5), IE(5),
     3                   XRR, RFC(9), KXR, NSTAGE, NCOMP, RMAX,
     4                   FTEST, STEST, NSPEC, NRHS, ISPEC(4), ISTAGE(4),
     5                   ICOMP(4), SPEC(4), JCTRL(4), NPRNT, MAX, NTIME,
     6                   K1, K2, K3, NL, NV, NPUNCH
C
      DIMENSION          KODE(4), DELFD(4), VALUE(4), TEST(4)
C
C
      NCHECK = 0
C
      WRITE ( K2, 8 )
    8 FORMAT (30H1DESIGN TO SPECIFICATION CHECK)
C
      DO  45   N=1,NSPEC
      KODE(N) = 0
      I = ISPEC(N)
      J = ISTAGE(N)
      K = ICOMP(N)
      L = JCTRL(N)
      DELFD(N) = 0.0
C
      GO TO ( 11, 12, 13, 14 ), I
C
C     RAFFINATE RATE                      SPECIFICATION # 1
   11 VALUE(N) = XL(J)
      TEST(N) = STEST
      M = NL
      GO TO 16
C
C     EXTRACT RATE                        SPECIFICATION # 2
   12 VALUE(N) = XV(J)
      TEST(N) = STEST
      M = NV
      GO TO 16
C
C     RAFFINATE COMPOSITION               SPECIFICATION # 3
   13 VALUE(N) = X(K,J)
      TEST(N) = FTEST
      M = K
      GO TO 16
C
```

```
C     EXTRACT COMPOSITION                        SPECIFICATION # 4
   14 VALUE(N) = Y(K,J)
      TEST(N) = FTEST
      M = K+NCOMP
C
   16 IF ( ABS(VALUE(N)-SPEC(N))/SPEC(N) .LT. TEST(N) ) KODE(N) = 1
C
C     CONTROL IS FEED NUMBER L
   18 IF ( KODE(N) .NE. 0 ) GO TO 19
      DELFD(N) = (SPEC(N)-VALUE(N))/(D(M,J,N+1)-D(M,J,1))
   19 OLD = FD(L)
      ZNEW = FD(L) + DELFD(N)
C
C     COMPUTE LOCATION OF MAXIMUM FLOW RATIO
C
   20 IF ( KODE(N) .NE. 0 ) GO TO 37
      NNN = 0
      LV = 0
      RATIO = 0.0
      DO  24   NN=1,NSTAGE
      DFLOW = ABS((D(NL,NN,N+1)-D(NL,NN,1))*DELFD(N))/XL(NN)
      IF ( DFLOW .LE. RATIO ) GO TO 23
      NNN = NN
      LV = 1
      RATIO = DFLOW
   23 DFLOW = ABS((D(NV,NN,N+1)-D(NV,NN,1))*DELFD(N))/XV(NN)
      IF ( DFLOW .LE. RATIO ) GO TO 24
      NNN = NN
      LV = 1
      RATIO = DFLOW
   24 CONTINUE
C
C     CHECK TO SEE IF NEW VALUE OF CONTROL VALUE NEEDS TO BE MODIFIED
C
   29 IF ( RATIO .GT. RMAX ) GO TO 30
      ZUSED = ZNEW
      GO TO 31
   30 FACTOR = RMAX/RATIO
      ZUSED = FD(L) + DELFD(N)*FACTOR
   31 FD(L) = ZUSED
      FAC = ZUSED/OLD
      DO  32   JJ=1,NCOMP
      FX(JJ,L) = FX(JJ,L)*FAC
   32 CONTINUE
C
C     SCALE CORRECTIONS TO FLOW RATES BASED ON (ZUSED-OLD)
C
      FAC = ZUSED-OLD
   35 DO  36   NN=1,NSTAGE
      D(NL,NN,1) = (D(NL,NN,N+1)-D(NL,NN,1))*FAC
      D(NV,NN,1) = (D(NV,NN,N+1)-D(NV,NN,1))*FAC
   36 CONTINUE
      GO TO 40
   37 ZUSED = ZNEW
C
   40 WRITE ( K2, 41 ) I, L, SPEC(N), VALUE(N), OLD, DELFD(N), ZNEW,
     1                 ZUSED
   41 FORMAT (/////5X18HSPECIFICATION TYPE I7 / 5X 12HCONTROL CODE I13
     1//5X19HSPECIFICATION VALUE1PE21.6/ 5X13HCURRENT VALUE1PE27.6 //
     25X24HPRESENT VALUE OF CONTROL0PF26.6/ 5X30HCOMPUTED CORRECTION TO
     3CONTROL F20.6 / 5X 26HESTIMATED VALUE OF CONTROL F24.6 / 5X 22HFIN
     4AL VALUE OF CONTROL F28.6 )
   45 CONTINUE
C
      DO  52   N=1,NSPEC
      IF ( KODE(N) .EQ. 0 ) GO TO 999
   52 CONTINUE
      NCHECK = 1
C
  999 RETURN
      END
      SUBROUTINE    PUNCH
C
      COMMON   /LIQEXT/  B(20,20), A(20,20), C(20,20,29), D(20,30,5),
     1                   XL(30), XV(30), X(9,30), Y(9,30), FD(7),
     2                   FX(9,8), IFX(7), R(5), IR(5), E(5), IE(5),
     3                   XKR, REC(9), KXR, NSTAGE, NCOMP, RMAX,
     4                   FTEST, STEST, NSPEC, NRHS, ISPEC(4), ISTAGE(4),
     5                   ICOMP(4), SPEC(4), JCTRL(4), NPRNT, MAX, NTIME,
     6                   K1, K2, K3, NL, NV, NPUNCH
C
      REAL               OUT(9)
      EQUIVALENCE        (OUT,B)
C
C
C     PUNCH OUT FLOW RATES
C
      DO  24   LV=1,2
      NN = NSTAGE/9
      IF ( MOD(NSTAGE,9) .GT. 0 ) NN=NN+1
      DO  23   N=1,NN
      J1 = (N-1)*9 + 1
      IF ( N .EQ. NN ) GO TO 12
      J2 = N*9
      GO TO 15
   12 J2 = NSTAGE
   15 DO  18   J=J1,J2
      K = J-J1+1
      GO TO ( 16, 17 ), LV
   16 OUT(K) = XL(J)
      GO TO 18
   17 OUT(K) = XV(J)
   18 CONTINUE
      LL = J2-J1+1
      WRITE ( K3, 21 ) (OUT(L),L=1,LL)
   21 FORMAT (9F8.2)
   23 CONTINUE
   24 CONTINUE
C
C     PUNCH OUT COMPOSITIONS
C
      DO  35   LV=1,2
      DO  34   N=1,NSTAGE
      DO  29   J=1,NCOMP
      GO TO ( 26, 27 ), LV
   26 OUT(J) = X(J,N)
      GO TO 29
   27 OUT(J) = Y(J,N)
   29 CONTINUE
      WRITE ( K3, 31 ) (OUT(L),L=1,NCOMP)
   31 FORMAT (9F8.6)
```

```
1171      34 CONTINUE
1172      35 CONTINUE
1173 C
1174         RETURN
1175         END
```

```
1176         SUBROUTINE    CLEAR ( A, N )
1177 C
1178         REAL     A(1)
1179 C
1180         DO  10   J=1,N
1181         A(J) = 0.0
1182      10 CONTINUE
1183 C
1184         RETURN
1185         END
```

```
      SUBROUTINE  ACTO ( II )
C
C     SUBROUTINE "ACTO"
C
C     EQUILIBRIUM DATA USING THE FOUR-SUFFIX MARGULES EQUATION FOR A
C     TERNARY SYSTEM
C
      COMMON   /LIQEXT/  B(20,20), A(20,20), C(20,20,29), D(20,30,5),
     1                   XL(30), XV(30), X(9,30), Y(9,30), FD(7),
     2                   FX(9,8), IFX(7), R(5), IR(5), E(5), IE(5),
     3                   XRR, REC(9), KXR, NSTAGE, NCOMP, RMAX,
     4                   FTEST, STEST, NSPEC, NRHS, ISPEC(4), ISTAGE(4),
     5                   ICOMP(4), SPEC(4), JCTRL(4), NPRNT, MAX, NTIME,
     6                   K1, K2, K3, NL, NV, NPUNCH
C
      COMMON   /EQDATA/  ACT(9,2), GAM(9,2), PGAM(9,9,2)
C
      COMMON   /AAZZ/    AA(9,9), DD(9), CC(9), JZ(9), ZZ(9)
C
C
      IF ( NTIME .NE. 0 ) GO TO 15
      CALL CLEAR ( AA, 117 )
      DO  3    J=1,NCOMP
      READ ( K1, 2 ) (AA(J,K),K=1,NCOMP)
    2 FORMAT (9F8.4)
    3 CONTINUE
      READ ( K1, 2 ) (DD(J),J=1,NCOMP)
      READ ( K1, 2 ) (CC(J),J=1,NCOMP)
C
      CSUM = 0.0
      DSUM = 0.0
      DO  4    K=1,NCOMP
      CSUM = CSUM + CC(K)
      DSUM = DSUM + DD(K)
    4 CONTINUE
C
      IF ( DSUM .EQ. 0.0 ) GO TO 5
      ASSIGN 33 TO M1
      ASSIGN 43 TO M3
      ASSIGN 53 TO M5
      ASSIGN 63 TO M7
      GO TO 6
    5 ASSIGN 34 TO M1
      ASSIGN 44 TO M3
      ASSIGN 54 TO M5
      ASSIGN 64 TO M7
C
    6 IF ( CSUM .EQ. 0.0 ) GO TO 7
      ASSIGN 35 TO M2
      ASSIGN 45 TO M4
      ASSIGN 55 TO M6
      ASSIGN 65 TO M8
      GO TO 8
    7 ASSIGN 36 TO M2
      ASSIGN 51 TO M4
      ASSIGN 61 TO M6
      ASSIGN 71 TO M8
C
    8 NTIME = 1
C
   15 I = II
      CALL CLEAR ( ACT, 198 )
C
      DO  98   LV=1,2
C
   17 DO 95    J=1,NCOMP
C
      JZ(1) = J
      DO 18    K=2,NCOMP
      JZ(K) = JZ(K-1) + 1
      IF ( JZ(K) .LE. NCOMP ) GO TO 18
      JZ(K) = JZ(K) - NCOMP
   18 CONTINUE
C
C     INITIALIZE COMPOSITIONS
C
      GO TO ( 19, 21 ), LV
C     RAFFINATE PHASE
   19 DO 20    K=1,NCOMP
      JJ = JZ(K)
      ZZ(K) = X(JJ,I)
   20 CONTINUE
      GO TO 27
C     EXTRACT PHASE
   21 DO 22    K=1,NCOMP
      JJ = JZ(K)
      ZZ(K) = Y(JJ,I)
   22 CONTINUE
C
   27 J1 = JZ(1)
      J2 = JZ(2)
      J3 = JZ(3)
      Z1 = ZZ(1)
      Z2 = ZZ(2)
      Z3 = ZZ(3)
C
   28 A12 = AA(J1,J2)
      A23 = AA(J2,J3)
      A31 = AA(J3,J1)
      A21 = AA(J2,J1)
      A32 = AA(J3,J2)
      A13 = AA(J1,J3)
      D12 = DD(J1)
      D23 = DD(J2)
      D31 = DD(J3)
      C1  = CC(J1)
      C2  = CC(J2)
      C3  = CC(J3)
C
C     COMPUTE ACTIVITY COEFFICIENT AND ACTIVITY
C
   31 ALNGAM = Z2**2 * ( A12 + 2.0*Z1*(A21-A12) )
     1       + Z3**2 * ( A13 + 2.0*Z1*(A31-A13) )
     2       + Z2 * Z3 * ( A21 + A13 - A32 +
     3                     2.0*Z1*(A31-A13) +
     4                     2.0*Z3*(A32-A23) )
   32 GO TO M1, ( 33, 34 )
   33 ALNGAM = ALNGAM  +  Z1 * Z2**2 * (3.0*Z1 - 2.0) * D12
     1       + 3.0 * Z2**2 * Z3**2 * D23
     2       + Z1 * Z3**2 * (3.0*Z1 - 2.0) * D31
   34 GO TO M2, ( 35, 36 )
   35 ALNGAM = ALNGAM  +  Z1 * Z2 * Z3 * (2.0 - 3.0*Z1) * C1
     1       - Z2**2 * Z3 * (1.0 - 3.0*Z1) * C2
     2       - Z2 * Z3**2 * (1.0 - 3.0*Z1) * C3
C
   36 GAM(J,LV) = 10.0**ALNGAM
      ACT(J,LV) = GAM(J,LV) * Z1
C
C     COMPUTE PARTIAL DERIVATIVES OF ACTIVITY COEFFICIENT
C
   41 PLGMZ1 = Z2**2 * 2.0 * (A21 - A12)
     1       + Z3 * (Z3 + Z2) * 2.0 * (A31 - A13)
   42 GO TO M3, ( 43, 44 )
   43 PLGMZ1 = PLGMZ1 + Z2**2 * (6.0*Z1 - 2.0) * D12
     1       + Z3**2 * (6.0*Z1 - 2.0) * D31
   44 GO TO M4, ( 45, 51 )
   45 PLGMZ1 = PLGMZ1 + Z2 * Z3 * (2.0 - 6.0*Z1) * C1
C
   51 PLGMZ2 = 2.0 * Z2 * ( A12 + 2.0*Z1*(A21-A12) )
     1       + Z3 * ( A21 + A13 - A32 +
     2                2.0*Z1*(A31-A13) +
     3                2.0*Z3*(A32-A23) )
   52 GO TO M5, ( 53, 54 )
   53 PLGMZ2 = PLGMZ2 + 2.0 * Z1 * Z2 * (3.0*Z1 - 2.0) * D12
     1       + 6.0 * Z2 * Z3**2 * D23
   54 GO TO M6, ( 55, 61 )
   55 PLGMZ2 = PLGMZ2 + Z1 * Z3 * (2.0 - 3.0*Z1) * C1
     1       - Z3 * (1.0 - 3.0*Z1) * (2.0*Z2*C2 + Z3*C3)
C
   61 PLGMZ3 = 3.0 * Z3 * ( A13 + 2.0*Z1*(A31-A13) )
```

```
C     1        + Z3 * (A21 - A32)
      2        + 2.0 * Z3 * (Z3 + Z2) * (A32 - A23)
   62 GO TO M7, ( 63, 64 )
   63 PLGMZ3 = PLGMZ3 + 6.0 * Z2**2 * Z3 * D23
      1        + 2.0 * Z1 * Z3 * (3.0*Z1 - 2.0) + D31
   64 GO TO M8, ( 65, 71 )
   65 PLGMZ3 = PLGMZ3 + Z1 * Z2 * (2.0 - 3.0*Z1) * C1
      1        - Z2 * (1.0 - 3.0*Z1) * (Z2*C2 + 2.0*Z3*C3)
C
   71 GO TO ( 74, 75, 76 ), J1
   74 PGAM(J,1,LV) = PLGMZ1
      PGAM(J,2,LV) = PLGMZ2
      PGAM(J,3,LV) = PLGMZ3
      GO TO 91
   75 PGAM(J,1,LV) = PLGMZ3
      PGAM(J,2,LV) = PLGMZ1
      PGAM(J,3,LV) = PLGMZ2
      GO TO 91
   76 PGAM(J,1,LV) = PLGMZ2
      PGAM(J,2,LV) = PLGMZ3
      PGAM(J,3,LV) = PLGMZ1
   91 DO  93   K=1,NCOMP
      PGAM(J,K,LV) = PGAM(J,K,LV) * GAM(J,LV) / 0.43429448
   93 CONTINUE
C
   95 CONTINUE
C
   98 CONTINUE
C
   99 RETURN
      END
```

I. PROBLEM IDENTIFICATION

1. Title: Batch Distillation
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II. TECHNICAL DESCRIPTION

1. Problem Statement: A binary mixture is to be distilled on a batch operation. It is desired to determine the variation of the pot composition when operating under conditions of variable or constant reflux ratios. The distillate yield and the total quantity of vapor are to be calculated simultaneously.

2. Problem Formulation and Technical Analysis: Batch distillation is normally used for separating small quantities of products. It is an unsteady-state operation that is usually carried in an existing column so that the number of plates is a given parameter. The necessary distillate composition can be achieved through two different distillation policies. In one, the composition is kept constant so that the reflux is varied, and in the second, the desired final composition is achieved through an averaging procedure of variable head composition at constant reflux ratio.

The discussion that follows will neglect the effect of hold-up on the quantity of liquid and vapor necessarily present in the plates of the column and in the condensers.

Policy A: Constant distillate composition - Variable reflux ratio.

The relation between the amount distilled D and the quantity of liquid W remaining in the kettle for an initial charge F may be calculated by a material balance. At any time during the process,

$$F = D + W \tag{1}$$

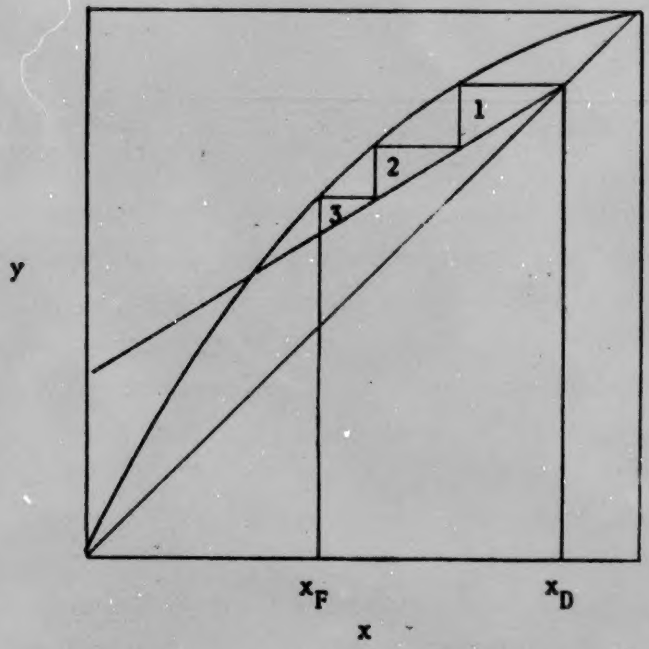
$$Fx_F = Dx_D + Wx_W \tag{2}$$

No feed is added, so that the entire column is an enriching section. Only the upper operating line exists

$$y_{n+1} = \frac{R}{R+1} x_n + \frac{x_D}{R+1} \qquad (3)$$

where y_{n+1} and x_n are the compositions of the vapor and liquid flowing past each other between stages, when the reflux ratio is R.

Equation (3) is used to determine the minimum reflux ratio that can be used. The operating line is located by trial so that the number of given plates will be the number of steps necessary to go from the distillate composition x_D to the initial feed x_F .



As soon as distillate begins to be withdrawn, the pot liquid becomes leaner, so that a higher reflux ratio is required to maintain the overhead composition. A new operating line is drawn, and the new pot composition is found, by stepping down the required number of plates. The procedure is continued until a reflux ratio is achieved that is un-economical.

The values of x_W and x_D allow the calculation of the corresponding values of W and D for every reflux ratio.

The total quantity of vapor G to be boiled up through the tower can be calculated by a material balance,

$$dG = \frac{R}{R+1} dG + dD \tag{4}$$

$$G = \int_0^D \frac{dD}{1- \frac{R}{R+1}} \tag{5}$$

and using equations (1) and (2)

$$G = F(x_D-x_F) \cdot \int_{x_{W_f}}^{x_F} \frac{dx_W}{(x_D-x_W)^2(1- \frac{R}{R+1})} \tag{6}$$

Equation (6) must be integrated graphically. The value of G is important because it is directly related to the heat cost of the process.

Policy B: Variable distillate composition - Constant reflux ratio.

It is possible to obtain a given distillate composition by running the column at a constant reflux ratio. Necessarily, the initial distillate will have to be richer than that of the overhead desired so that averaging with more dilute product will produce the final product.

The graphical procedure is exactly the same as before, except that an averaging equation must be added to determine the end of the process.

A material balance at any time gives

$$Wx_W = x_D dW + (W-dW)(x_W-dx_W) \tag{7}$$

$$\ln \frac{F}{W} = \ln \frac{W}{W_0} = \int_{x_{W_f}}^{x_F} \frac{dx_W}{x_D-x_W} \tag{8}$$

Graphical solution of this equation will permit calculation of the fraction of the initial load, W/W_0 , that has to be distilled in order to achieve the average overhead composition desired.

For high product concentration the operating line will have to be shifted closer to the azeotropic point or to the point (1.1). This impairs seriously the precision of the graphical method, and alternative ways have to be used for drawing the stages.

3. Method of Solution: There are minor differences between the two policies.

The number of plates can be stepped down the operating line using a straight-line interpolation of the vapor-liquid equilibrium data.

If the increment steps for advancing the reflux ratio or the starting point of the operating line are kept sufficiently small, enough points can be obtained to perform the integration of equations (6) and (8) by successive quadrature of the new point added, without recourse to other integrating techniques.

4. References and Data: The problem requires a basic knowledge of distillation such as given in any standard Unit Operations book. Equilibrium data may be obtained from Table 13-3 in Perry's Handbook.

5. Solution: The computer output entitled "Batch distillation with negligible hold-up" tabulates for every reflux ratio, the pot composition, fraction evaporated, and ratio of total vapor to initial load.

III. EDUCATIONAL (PEDAGOGICAL) ASPECTS

1. Description of Past Usage: The problem has been sparsely used in a Unit Operation course for Juniors.

2. Concept Demonstrated: a) Integration by quadrature, b) Linear interpolation.

Evaluation of Usage: This is a four-week assignment. Students may be required to compare both methods on a cost basis and suggest a distillation policy.

IV. PROGRAM SUMMARY SHEET

```
C     BATCH DISTILLATION WITH NEGLIGIBLE HOLD-UP AND REFLUX CONSTANT OR MAIN0001
C     VARIABLE.                                                         MAIN0002
C****                                                                   MAIN0003
C     DESCRIPTION OF MAIN VARIABLES                                     MAIN0004
C****                                                                   MAIN0005
C     DELTA.-  INCREMENT FOR ADVANCING THE OPERATING LINE               MAIN0006
C                                                                       MAIN0007
C     FRAC.-   FRACTION OF INITIAL LOAD DISTILLED                       MAIN0008
C                                                                       MAIN0009
C     KOLOR.-  CONTROL CARD TO INDICATE END OF DATA.LAST SET OF DATA    MAIN0010
C              HAS A POSITIVE NUMBER IN COLUMN 70 OF FIRST CARD         MAIN0011
C                                                                       MAIN0012
C     NM.-     NUMBER OF POINTS.EQUILIBRIUM DATA                        MAIN0013
C                                                                       MAIN0014
C     NP.-     NUMBER OF THEORETICAL PLATES                             MAIN0015
C                                                                       MAIN0016
C     R.-      REFLUX RATIO                                             MAIN0017
C                                                                       MAIN0018
C     RMAX.-   MAXIMUM REFLUX RATIO ALLOWED                             MAIN0019
C                                                                       MAIN0020
C     S.-      VECTOR IDENTIFYING THE COMPONENTS                        MAIN0021
C                                                                       MAIN0022
C     VAPOR.-  RATIO OF TOTAL VAPOR GENERATED TO INITIAL LOAD           MAIN0023
C                                                                       MAIN0024
C     X.-      MOLE OR WEIGHT FRACTION IN LIQUID IN PLATE N             MAIN0025
C                                                                       MAIN0026
C     XAZEO.-  MOLE OR WEIGHT FRACTION IN AZEOTROPE IF PRESENT. ITS     MAIN0027
C              VALUE IS 1.0 WHEN NO AZEOTROPE IS PRESENT                MAIN0028
C                                                                       MAIN0029
C     XWF.-    FINAL POT COMPOSITION                                    MAIN0030
C                                                                       MAIN0031
C     XDM.-    MOLE OR WEIGHT FRACTION DESIRED IN THE DISTILLATE        MAIN0032
C                                                                       MAIN0033
C     XWO.-    MOLE OR WEIGHT FRACTION IN INITIAL SOLUTION              MAIN0034
C                                                                       MAIN0035
```

```
C     XX.-      EQUILIBRIUM COMPOSITION IN LIQUID                         MAIN0036
C                                                                         MAIN0037
C     Y.-       MOLE OR WEIGHT FRACTION OF VAPOR IN PLATE N               MAIN0038
C                                                                         MAIN0039
C     YY.-      EQUILIBRIUM COMPOSITION IN VAPOR                          MAIN0040
C****                                                                     MAIN0041
C     DATA INPUT                                                          MAIN0042
C                                                                         MAIN0043
C                         VARIABLES                  FORMAT               MAIN0044
C                                                                         MAIN0045
C     FIRST CARD          NP,MM,XDM,XAZEO,           2I13,4F10.5,I10      MAIN0046
C                         RMAX,KOLOR                                      MAIN0047
C                                                                         MAIN0048
C     SECOND CARD         YY(N),XX(N)                2F10.5               MAIN0049
C                                                                         MAIN0050
C     THIRD CARD          S                          15A4                 MAIN0051
C                                                                         MAIN0052
C**** LIMITATIONS.-                                                       MAIN0053
C     ALL COMPOSITIONS ARE BASED ON THE LIGHT COMPONENT. VAPOR-LIQUID     MAIN0054
C     EQUILIBRIUM DATA MUST BE ARRANGED FROM (0,0) ON TO AZEOTROPE OR     MAIN0055
C     POINT (1,1)                                                         MAIN0056
C****                                                                     MAIN0057
C     OUTPUT                                                              MAIN0058
C     IN BOTH CASES FOR EVERY REFLUX RATIO, THE POT COMPOSITION,          MAIN0059
C     FRACTION EVAPORATED,AND RATIO OF TOTAL VAPOR TO INITIAL LOAD        MAIN0060
C                                                                         MAIN0061
C                                                                         MAIN0062
      DIMENSION X(30),Y(30),YY(30),XX(30),S(15)                           MAIN0063
      DATA IN,IO/5,6/                                                     MAIN0064
C     THE VALUE OF XAZEO IS 1.0 OR THE AZEOTROPIC COMPOSITION.            MAIN0065
C     RMAX POSITIVE CORRESPONDS TO THE CASE OF CONSTANT REFLUX RATIO.     MAIN0066
C     DISTILLATION DATA                                                   MAIN0067
  100 READ(IN,400)NP,MM,XW0,XDM,XAZEO,RMAX,KOLOR
C     VAPOR-LIQUID EQUILIBRIUM DATA FROM A SMOOTHED CURVE                 MAIN0069
```

```
      DC 101 N=1,MM                                                     MAIN0070
  101 READ(IN,402) YY(N),XX(N)                                          MAIN0071
C     IDENTIFICATICN OF THE SYSTEM                                      MAIN0072
      READ(IN,405) S                                                    MAIN0073
      IF(RMAX)200,200,105                                               MAIN0074
C     THIS PCRTICN CF THE PRCGRAM CORRESPONDS TO CONSTANT REFLUX.       MAIN0075
  105 WRITE(IO,410) S,XWO,XCM,NP                                        MAIN0076
C     THE VALUE OF A DETERMINES THE SIZE OF THE INTEGRATICN STEP.       MAIN0077
      A=XAZEC-0.03                                                      MAIN0078
C     THE VALUE OF BU LIMITS THE APPLICATION  OF THE METHCD.            MAIN0079
      BU=RMAX                                                           MAIN0080
      GC TC 138                                                         MAIN0081
C     THE CALCULATING PROCEDURE STARTS WITH THE MAXIMUM REFLUX  RATIC   MAIN0100
C     ASSIGNED. IT IS DECREASED UNTIL IT IS NOT SUFFICIENT FCR THE      MAIN0101
C     NUMBER OF PLATES AVAILABLE.                                       MAIN0102
  138 R=10.*RMAX+1.                                                     MAIN0103
      IR=R                                                              MAIN0104
  500 DC 190 KR=1,IR,5                                                  MAIN0105
      MR=IR-KR                                                          MAIN0106
      R=MR                                                              MAIN0107
      R=0.1*R                                                           MAIN0108
      K=1                                                               MAIN0109
      Y(1)=XCM                                                          MAIN0110
      XP=XCM                                                            MAIN0111
      M=1                                                               MAIN0112
C     LINEAR INTERPOLATION OF EQUILIBRIUM DATA                          MAIN0082
  115 DC 136 K=1,NP                                                     MAIN0083
      IF(Y(K)-YY(2))120,122,124                                         MAIN0084
  120 X(K)=XX(1)+(XX(2)-XX(1))*(Y(K)-YY(1))/(YY(2)-YY(1))               MAIN0085
      GC TC 134                                                         MAIN0086
  122 X(K)=XX(2)                                                        MAIN0087
      GC TC 134                                                         MAIN0088
  124 N=3                                                               MAIN0089
  126 IF(Y(K)-YY(N))132,128,130                                         MAIN0090
  128 X(K)=XX(N)                                                        MAIN0091
      GC TC 134                                                         MAIN0092
      130 N=N+1                                                            MAIN0093
          GC TC 126                                                        MAIN0094
      132 PEND=(XX(N)-XX(N-1))/(YY(N)-YY(N-1))                             MAIN0095
          X(K)=XX(N-1)+PEND*(Y(K)-YY(N-1))                                 MAIN0096
      134 Y(K+1)=R*X(K)/(R+1.)+XP/(R+1.)                                   MAIN0097
      136 CCNTINUE                                                         MAIN0098
          GC TC(140,146,174),M                                             MAIN0099
C         CHECK THAT IT IS POSSIBLE TO RECTIFY UNDER GIVEN CONDITIONS     MAIN0114
      140 IF(X(K-1)-XW0) 142,192,192                                       MAIN0115
      142 FU2=0.                                                           MAIN0116
          XW2=0.                                                           MAIN0117
          XWA=X(K-1)                                                       MAIN0118
          FA=1./(XDM-XWA)                                                  MAIN0119
          J=1                                                              MAIN0120
          XDT=XCM+0.01                                                     MAIN0121
C         INTERPCLATICN PROCEDURE                                          MAIN0122
      144 K=1                                                              MAIN0123
          Y(1)=XDT                                                         MAIN0124
          XP=XCT                                                           MAIN0125
          M=2                                                              MAIN0126
          GC TC 115                                                        MAIN0127
      146 IF(X(K-1)-XW0) 150,150,170                                       MAIN0128
      150 IF(J-1) 152,152,151                                              MAIN0129
      151 F1=F2                                                            MAIN0130
C         INTEGRATION BY QUADRATURE                                        MAIN0131
          F2=1./(XDT-X(K-1))                                               MAIN0132
          SUMA=SUMA+0.5*(F1+F2)*(XW2-X(K-1))                               MAIN0133
          GC TC 154                                                        MAIN0134
      152 F2=1./(XDT-X(K-1))                                               MAIN0135
          SUMA=0.5*(FA+F2)*(XWA-X(K-1))                                    MAIN0136
          J=2                                                              MAIN0137
      154 XW2=X(K-1)                                                       MAIN0138
          IF(XCT-A) 156,156,158                                            MAIN0139
      156 XDT=XCT+0.01                                                     MAIN0140
          GC TC 144                                                        MAIN0141
      158 DELTA=0.002                                                      MAIN0142
          IF(XCT-0.999) 162,160,160                                        MAIN0143
```

```
  160 DELTA=0.0001                                                      MAIN0144
  162 XDT=XCT+DELTA                                                     MAIN0145
      IF(XCT-XAZEC) 144,196,196                                         MAIN0146
  170 F1=F2                                                             MAIN0147
      F2=F1+(1./(XCT-X(K-1))-F1)*(XW0-XW2)/(X(K-1)-XW2)                 MAIN0148
      SUMA=SUMA+0.5*(F1+F2)*(XW2-XW0)                                   MAIN0149
      XCTU=XCT                                                          MAIN0150
      XDT=XCM                                                           MAIN0151
      F1=FA                                                             MAIN0152
      XW2=XWA                                                           MAIN0153
  172 XDT=XCT-0.4*(XCTU-XCM)                                            MAIN0154
      K=1                                                               MAIN0155
      Y(1)=XCT                                                          MAIN0156
      XP=XCT                                                            MAIN0157
      M=3                                                               MAIN0158
      GC TC 115                                                         MAIN0159
  174 F2=1./(XDT-X(K-1))                                                MAIN0160
      SUMA=SUMA+0.5*(F1+F2)*(X(K-1)-XW2)                                MAIN0161
      PLCG=ALOG((XDM-XW0)/(XDM-X(K-1)))                                 MAIN0162
      FU1=FL2                                                           MAIN0163
      FU2=SUMA-PLCG                                                     MAIN0164
      IF(FU2) 178,180,176                                               MAIN0165
  176 F1=F2                                                             MAIN0166
      XW2=X(K-1)                                                        MAIN0167
      GC TC 172                                                         MAIN0168
C     MATERIAL BALANCE TO DETERMINE END POINT                           MAIN0169
  178 XWF=(FU1*X(K-1)-FU2*XW2)/(FU1-FU2)                                MAIN0170
      GC TC 182                                                         MAIN0171
  180 XWF=X(K-1)                                                        MAIN0172
  182 FRAC=(XW0-XWF)/(XDM-XWF)                                          MAIN0173
      VAPOR=(1.+R)*FRAC                                                 MAIN0174
C     PRINT REFLUX RATIO,POT CONCENTRATION,FRACTICN DISTILLED AND       MAIN0175
C     VAPOR GENERATEC                                                   MAIN0176
      WRITE(IO,415)R,XWF,FRAC,VAPOR                                     MAIN0177
  190 CCNTINUE                                                          MAIN0178
      GCTC 390                                                          MAIN0179
C     MESSAGE THAT NUMBER OF PLATES IS INSUFFICIENT                     MAIN0180
```

```
  192 WRITE(IO,420)R                                                    MAIN0181
      IF(BU-RMAX)194,390,390                                            MAIN0182
C     MESSAGE THAT METHOD FAILS TO BE PRECISE                           MAIN0183
  194 WRITE(IO,425)BU                                                   MAIN0184
      GCTC 390                                                          MAIN0185
  196 BU=R                                                              MAIN0186
      GC TC 500                                                         MAIN0187
C     THIS FCRTICN OF THE PROGRAM CORRESPONDS TO VARIABLE REFLUX.       MAIN0188
  200 WRITE(IO,430)S,XWO,XDM,NP                                         MAIN0189
C     DETERMINATION CF MINIMUM OPERATING REFLUX RATIC                   MAIN0190
      ALFA=XDM-XWO                                                      MAIN0191
      Y(1)=XDM                                                          MAIN0192
      N=1                                                               MAIN0193
  210 IF(XWO-XX(N+1))216,214,212                                        MAIN0194
  212 N=N+1                                                             MAIN0195
      GCTO 210                                                          MAIN0196
  214 YWO=YY(N+1)                                                       MAIN0197
      GCTC 218                                                          MAIN0198
  216 YWO=YY(N)+(YY(N+1)-YY(N))*(XWO-XX(N))/(XX(N+1)-X(N))              MAIN0199
  218 PEND=(XDM-YWO)/ALFA                                               MAIN0200
      IF(PEND)350,220,220                                               MAIN0201
  220 IRT=10.*PEND/(1.-PEND)                                            MAIN0202
      R=IRT+1                                                           MAIN0203
      R=0.1*R                                                           MAIN0204
      M=1                                                               MAIN0205
  230 DC 248 K=1,NP                                                     MAIN0206
      N=1                                                               MAIN0207
  234 IF(Y(K)-YY(N+1))240,238,236                                       MAIN0208
  236 N=N+1                                                             MAIN0209
      GCTC 234                                                          MAIN0210
  238 X(K)=XX(N+1)                                                      MAIN0211
      GCTO 242                                                          MAIN0212
  240 P=(XX(N)-XX(N+1))/(YY(N)-YY(N+1))                                 MAIN0213
      X(K)=XX(N)+P*(Y(K)-YY(N))                                         MAIN0214
  242 Y(K+1)=R*X(K)/(1.+R)+XDM/(1.+R)                                   MAIN0215
  248 CCNTINUE                                                          MAIN0216
      GC TC (250,285),M                                                 MAIN0217
  250 IF(X(K-1)-XWO)254,254,252                                         MAIN0218
  252 XW1=X(K-1)                                                        MAIN0219
```

```
C       THE REFLUX RATIO IS INCREASED IN VARIABLE STEPS UP TO A MAXIMUM   MAIN0220
C       VALUE CF 20                                                       MAIN0221
        R=R+0.1                                                           MAIN0222
        GCTC 230                                                          MAIN0223
  254   R=R-0.1+0.1*(XW1-XW0)/(XW1-X(K-1))                                MAIN0224
C       INTEGRATICN BY QUADRATURE                                         MAIN0225
        F1=0.                                                             MAIN0226
        VAPOR=0.                                                          MAIN0227
        FRAC=0.                                                           MAIN0228
        XW2=XW0                                                           MAIN0229
        F2=ALFA/((1.-R/(1.+R))*(XDM-XW0)**2)                              MAIN0230
        WRITE(IO,415)R,XW2,FRAC,VAPOR                                     MAIN0231
        IR=R                                                              MAIN0232
C       REFLUX RATIO INCREASEC IN APPROPIATE STEPS                        MAIN0233
        IF(IR-5)256,260,260                                               MAIN0234
  256   Q=R                                                               MAIN0235
        R=IR                                                              MAIN0236
        R=R+0.5                                                           MAIN0237
        IF(R-C)258,280,280                                                MAIN0238
  258   R=R+0.5                                                           MAIN0239
        GCTC 280                                                          MAIN0240
  260   IF(IR-10)262,264,264                                              MAIN0241
  262   R=IR                                                              MAIN0242
        R=R+1.                                                            MAIN0243
        GCTC 280                                                          MAIN0244
C       REFLUX RATIO LIMITEC TO 20                                        MAIN0245
  264   IF(IR-20)266,355,355                                              MAIN0246
  266   R=IR                                                              MAIN0247
        R=R+2.                                                            MAIN0248
  280   R1=1.+R                                                           MAIN0249
        R2=R/(1.+R)                                                       MAIN0250
        R3=1.-R2                                                          MAIN0251
        R4=XCM/R1                                                         MAIN0252
        M=2                                                               MAIN0253
        GCTC 230                                                          MAIN0254
  285   F1=F2                                                             MAIN0255
        F2=ALFA/(R3*(XDM-X(K-1))**2)                                      MAIN0256
        XW1=XW2                                                           MAIN0257
```

```
      XW2=X(K-1)                                                        MAIN0258
      VAPOR=VAPOR+0.5*(F1+F2)*(XW1-XW2)                                 MAIN0259
      FRAC=(XW0-X(K-1))/(XDM-X(K-1))                                    MAIN0260
      WRITE(IO,415)R,XW2,FRAC,VAPOR                                     MAIN0261
      IF(R-5.)295,300,300                                               MAIN0262
  295 R=R+0.5                                                           MAIN0263
      GCTC 280                                                          MAIN0264
  300 IF(R-10.)320,330,330                                              MAIN0265
  320 R=R+1.                                                            MAIN0266
      GCTC 280                                                          MAIN0267
  330 IF(R-20.) 340,390,390                                             MAIN0268
  340 R=R+2.                                                            MAIN0269
      GCTC 280                                                          MAIN0270
  350 WRITE(IO,435)                                                     MAIN0271
      GCTC 390                                                          MAIN0272
C     MESSAGE THAT MAXIMUM REFLUX RATIO OF 20 IS NOT SUFFICIENT         MAIN0273
  355 WRITE(IO,440)                                                     MAIN0274
  390 IF(KCLCR)100,100,395                                              MAIN0275
  395 CALL EXIT                                                         MAIN0276
  400 FCRMAT(2I10,4F10.5,I10)                                           MAIN0277
  402 FCRMAT(2F10.5)                                                    MAIN0278
  405 FCRMAT(15A4)                                                      MAIN0279
  410 FORMAT(1H1,47HBATCH DISTILLATION WITH NEGLIGIBLE HOLD-UP AND ,    MAIN0280
     115HCCNSTANT REFLUX////,7H SYSTEM,21X,15A4/,19H INITIAL COMPOSITIO,MAIN0281
     21HN,F13.3/,24H DISTILLATE COMPOSITION,F9.3/,18H THEORETICAL PLATE,MAIN0282
     31HS,I12//,28X,7HRESULTS//,7H REFLUX,4X,7HRESIDUE,10X,8HFRACTION,  MAIN0283
     46X,12HTOTAL VAPOR//,6H RATIO,5X,13HCONCENTRATICN,4X,10HEVAPORATED,MAIN0284
     54X,12HINITIAL LOAD//)                                             MAIN0285
  415 FORMAT(1H ,F5.1,F11.3,F18.3,F15.3)                                MAIN0286
  420 FCRMAT(//40H FCR REFLUX RATIOS EQUAL OR SMALLER THAN,F5.1,5H THE ,MAIN0287
     116HNUMBER OF PLATES/,41H AVAILABLE IS NOT SUFFICIENT FOR OBTAININ,MAIN0288
     237HG THE DISTILLATE CCMPOSITION DESIRED.//)                       MAIN0289
  425 FORMAT(/39H FOR REFLUX RATIOS EQUAL OR LARGER THAN,F5.1,4HTHE ,   MAIN0290
     159HMETHOD IS NCT PRECISE BECAUSE THE OPERATING LINE STARTS TOO/,  MAIN0291
     250HCLCSE TO THE AZECTROPIC COMPOSITION OR POINT (1,1))            MAIN0292
```

```
   193      430 FORMAT(1H1,48H BATCH DISTILLATION WITH NEGLIGIBLE HOLD-UP AND ,    MAIN0293
               115HVARIABLE REFLUX////,7H SYSTEM,21X,15A4/,19H INITIAL COMPOSITIO,MAIN0294
               21HN,F13.3/,24H DISTILLATE COMPOSITION,F9.3/,18H THEORETICAL PLATE,MAIN0295
               31HS,I12//,28X,7HRESULTS//,7H REFLUX,4X,7HRESIDUE,10X,8HFRACTION,  MAIN0296
               46X,12HTOTAL VAPOR//,6H RATIO,5X,13HCONCENTRATION,4X,10HEVAPORATED,MAIN0297
               54X,12HINITIAL LOAD//)                                             MAIN0298
   194      435 FORMAT(//52H THE DISTILLATE COMPOSITION DESIRED IS SMALLER THAN , MAIN0299
               134HTHAT IN EQUILIBRIUM WITH THE FEED.///)                         MAIN0300
   195      440 FORMAT(///48H IN ORDER TO ACHIEVE THE DISTILLATE COMPOSITION ,    MAIN0301
               161HDESIRED IT IS NECESSARY TO OPERATE WITH REFLUX RATIOS LARGER , MAIN0302
               28HTHAN 20.)                                                       MAIN0303
   196          END                                                               MAIN0304
            C
            C*****DATA
**WARNING**  END STATEMENT NOT PRECEDED BY A TRANSFER

            $EXEC
```

```
BATCH DISTILLATICN WITH NEGLIGIBLE HOLC-UP AND CONSTANT REFLUX


SYSTEM                           ETHANCL-WATER
INITIAL CCMPCSITICN              0.200
DISTILLATE COMPOSITICN.          0.745
THEORETICAL PLATES                 4

                                 RESULTS

REFLUX     RESIDUE               FRACTION        TOTAL VAPOR/
RATIO      CCNCENTRATICN         EVAPORATED      INITIAL LOAD


 10.0        0.007                 0.261            2.873
  9.5        0.009                 0.260            2.727
  9.0        0.011                 0.258            2.578
  8.5        0.013                 0.255            2.424
  8.0        0.017                 0.251            2.261
  7.5        0.022                 0.246            2.092
  7.0        0.028                 0.240            1.920
  6.5        0.035                 0.233            1.744
  6.0        0.043                 0.223            1.562
  5.5        0.054                 0.211            1.370
  5.0        0.071                 0.191            1.147
  4.5        0.139                 0.100            0.551
  4.0        0.155                 0.076            0.380
  3.5        0.179                 0.036            0.163


FOR REFLUX RATIOS ECUAL OR SMALLER THAN  3.0 THE NUMBER OF PLATES
AVAILABLE IS NCT SUFFICIENT FOR OBTAINING THE DISTILLATE COMPOSITION DESIRED.
```

```
BATCH DISTILLATION WITH NEGLIGIBLE HOLD-UP AND VARIABLE REFLUX


SYSTEM                          CHLOROFORM-BENZENE
INITIAL COMPOSITION             0.360
DISTILLATE COMPOSITION.         0.960
THEORETICAL PLATES               10

                                RESULTS

REFLUX     RESIDUE              FRACTION        TOTAL VAPOR/
RATIO      CONCENTRATION        EVAPORATED      INITIAL LOAD


  3.7        0.360                0.000            0.000
  4.0        0.344                0.025            0.122
  4.5        0.326                0.054            0.273
  5.0        0.310                0.077            0.404
  6.0        0.285                0.112            0.629
  7.0        0.265                0.137            0.820
  8.0        0.248                0.157            0.988
  9.0        0.235                0.173            1.138
 10.0        0.223                0.186            1.273
 12.0        0.205                0.205            1.508
 14.0        0.191                0.219            1.706
 16.0        0.181                0.230            1.876
 18.0        0.172                0.238            2.027
 20.0        0.165                0.245            2.162
```

I. PROBLEM IDENTIFICATION

1. Title: Continuous Multistage Binary Distillation
2. Author: Alkis Constantinides
3. Affiliation: Rutgers University

II. TECHNICAL DESCRIPTION

1. Problem Statement: Write a computer program to perform the stage-to-stage calculations for a distillation column with the following feed and product specifications:

	propane	n-butane
Feed composition:	0.5	0.5
Distillate composition:	0.9	0.1
Bottoms composition:	0.1	0.9

Feed rate: 100 moles/hour

Thermal condition of feed: $q = 0.2$

Assume constant molar overflow in the distillation column. Use a total condenser and a partial reboiler. Assume that there is no entrainment from the reboiler and that the efficiency of the reboiler is 1.0. Use the following additional specifications:

Murphree Vapor Efficiency: Use $E_{MV} = 0.70$ in both sections of the column

Entrainment: $\varepsilon = 0.10$ in both sections of the column (ε = mole of liquid entrained per mole of vapor)

External Reflux Ratio: $\frac{L}{D} = 2.0$

Operating Pressure: 220 psia

Distribution Coefficients ($K = \frac{y}{x}$):

$$\ln K = \frac{A}{T} + B + CT$$

where T = absolute temperature, °R

at 220 psia the values of the constants are:

	A	B	C
propane	-3087.933	8.63131	-0.00290
n-butane	-4760.751	8.50187	-0.00206

This program should be used to solve the following cases:

a. Using the above information calculate:
   - i. Flow rates of all streams
   - ii. Bubble point temperatures of liquids from each stage (including reboiler)

   iii. Composition of liquid and vapor streams from each stage

   iv. Number of stages needed for the required separation

   v. On which stage (counting from the bottom of the column) is the feed introduced?

b. Repeat (a), but set the entrainment equal to 0.0 throughout the column. What effect does this have on the number of stages required?

c. Repeat (a), but set the efficiency equal to 1.0. What is the effect of this change?

d. Repeat (a), but use $\frac{L}{D} = 30.0$. What is the effect of this change? Why?

e. Repeat (a), but use $\frac{L}{D} = 1.5$. What is the effect of this change? Why?

2. Problem Formulation and Technical Analysis: The equations for the complete solution of this problem will be divided into the following six groups which will be discussed below: (a) External material balances around column and condenser, (b) Material balances around feed plate, (c) Material balance around reboiler, (d) Material balance in the stripping section, (e) Material balances in the enriching section, and (f) Feed flash and bubble-point claculations.

a. External material balances: The flow rates of distillate and bottoms are obtained from the external material balances on the column (Figure 1) resulting in the following two equations

$$D = \frac{F(z_F - x_W)}{(x_D - x_W)} \qquad (1)$$

$$W = F - D \qquad (2)$$

The liquid and vapor flow rates in the enriching section are obtained from the reflux ratio (L/D) and from a material balance around the condenser

$$L = (L/D)\ D \qquad (3)$$

$$V = L + D \qquad (4)$$

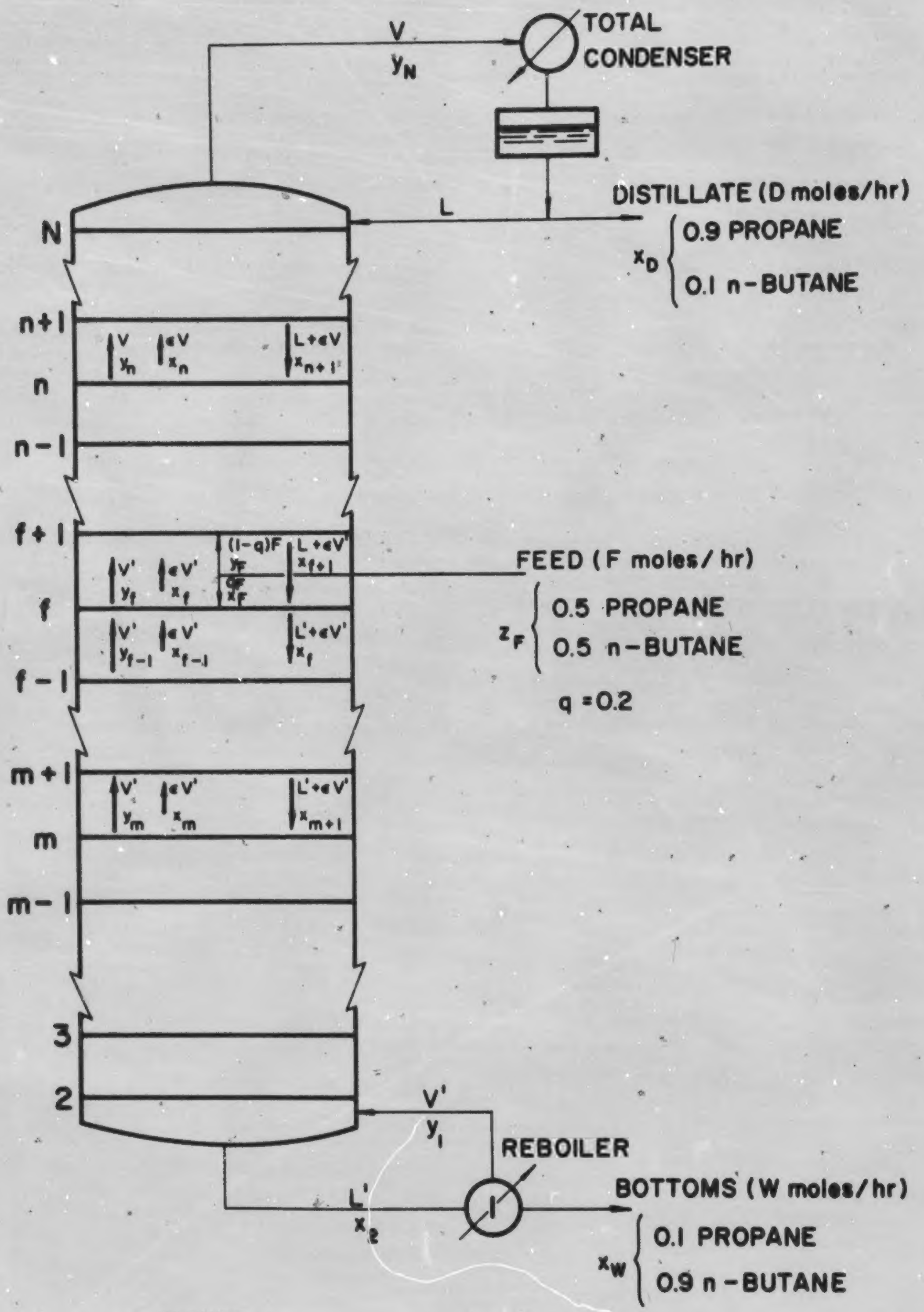

V
y_N
TOTAL CONDENSER
DISTILLATE (D moles/hr)
L
N
x_D
0.9 PROPANE
0.1 n-BUTANE
n+1
V
y_n
εV
x_n
L+εV
x_{n+1}
n
n-1
f+1
(1-q)F
y_F
qF
x_F
L+εV'
x_{f+1}
V'
y_f
εV'
x_f
FEED (F moles/hr)
f
z_F
0.5 PROPANE
0.5 n-BUTANE
V'
y_{f-1}
εV'
x_{f-1}
L'+εV'
x_f
f-1
q = 0.2
m+1
V'
y_m
εV'
x_m
L'+εV'
x_{m+1}
m
m-1
3
2
V'
y_1
REBOILER
L'
x_2
1
BOTTOMS (W moles/hr)
x_W
0.1 PROPANE
0.9 n-BUTANE

FIGURE 1

It is assumed that the liquid from the condenser is saturated liquid. It is also assumed that there is constant molar overflow in each section of the distillation column.

b. Balance around the feed plate: The values of L' and V' can be obtained by taking into account the thermal condition of the feed:

$$L' = L + qF \qquad (5)$$

$$V' = V - (1-q)F \qquad (6)$$

c. Balance around reboiler: All the quantities are now available for a balance around the reboiler. There is no entrainment from the reboiler and its efficiency is taken to be 1.0.

$$\therefore x_2 = \frac{(V'y_1 + Wx_W)}{L'} \qquad (7)$$

The value of y_1 is obtained from a bubble-point calculation to be described later. Note that the reboiler is counted as Stage No. 1 in the printout of the results.

d. Balance in stripping section: The concentration of the liquid from each stage in the stripping section is given by the material balance around the stripping section

$$x_{m+1} = \frac{(V'y_m + \varepsilon V'x_m) + Wx_W}{L' + \varepsilon V'} \qquad (8)$$

where y_m is calculated using the Murphree vapor efficiency

$$y_m = E_{MV}\,(y^*_m - y_{m-1}) + y_{m-1} \qquad (9)$$

and y^*_m is the composition of vapor in equilibrium with the liquid of composition x_m (y^*_m is determined by the bubble-point calculation).

e. Material balances in enriching section: The transfer between the stripping section and the enriching section is bridged by the equation resulting from a material balance right above the feed plate. This balance includes the vapor portion of the feed:

$$x_{f+1} = \frac{V'y_f + \varepsilon V'x_f + (1-q)Fy_F - Dx_D}{L + \varepsilon V'} \tag{10}$$

where the subscript f designates the feed plate. The composition of the liquid from the rest of the stages in the enriching section is given by the operating equation of this section:

$$x_{n+1} = \frac{(Vy_n + \varepsilon Vx_n) - Dx_D}{L + \varepsilon V} \tag{11}$$

where y_n and y_n^* are calculated as in the stripping section.

f. Feed flash and bubble-point calculations: There are two types of calculations performed:

i) Given the overall feed composition (z_F), assume a flash temperature T and calculate the values of K from

$$\ln K = \frac{A}{T} + B + CT \tag{12}$$

Using this value of K, calculate the compositions of the vapor and liquid resulting from the flashing of the feed:

$$y_F = \frac{z_F}{1 + q(\frac{1}{K} - 1)} \tag{13}$$

$$x_F = \frac{y_F}{K} \tag{14}$$

Calculate $\sum_i y_{F_i}$ for all components. Correct the values of y_F by:

$$y_F^{new} = \frac{y_F}{\sum_i y_{F_i}} \tag{15}$$

Calculate new values of K:

$$K_{new} = \frac{y_F^{new}}{x_F} \tag{16}$$

A Newton-Raphson technique is used to find the new flash temperature which satisfies equation (12) with the value K_{new}. The program continues to iterate around equations (12)-(16) until equation (17) is satisfied.

$$\sum_i y_{F_i} = 1.0 \tag{17}$$

ii) The bubble point for the reboiler and for each stage is obtained as follows: given the liquid composition (x_n), and an estimate of the bubble-point temperature (T) calculate K from equation (12) and y_n^* from

$$y_n^* = Kx_n \tag{18}$$

Calculate $\sum_i y_{n_i}^*$ for all components. Correct the values of y_n^* by

$$y_n^* = \frac{y_n^*}{\sum_i y_{n_i}^*} \tag{19}$$

Calculate new values of K

$$K_{new} = \frac{y_n^*}{x_n} \tag{20}$$

Using K_{new} in equation (12) find a new bubble-point temperature. Continue with corrections until

$$\sum_i y_{n_i}^* = 1.0 \tag{21}$$

is satisfied.

3. Method of Solution: The sequence of steps for the solution of this problem is essentially the following:

a. Solve equations (1) through (7) sequentially

b. Obtain the flash temperature of the feed and the composition of the vapor and liquid portions resulting from the flash (use equations (12)-(17)).

c. Proceed with the stage-to-stage calculations in the stripping section starting from the reboiler (use equations (8), (9) and the bubble-point calculations) until the temperature of the stage becomes lower than the feed flash temperature.

d. Shift to enriching section (use equation (10)) and proceed with stage-to-stage calculation (equations (11), (9) and bubble-point calculations) until the vapor composition coming off from a stage is higher than x_D in the light component.

4. References

B.D. Smith, "Design of Equilibrium Stage Processes," McGraw-Hill Book Company, New York (1963)

C.D. Holland, "Multicomponent Distillation," Prentice Hall, New Jersey (1963)

"Perry's Chemical Engineer's Handbook," 4th Edition, McGraw-Hill Book Company, New York (1963)

E.J. Henley and H.K. Staffin, "Stagewise Process Design," J. Wiley & Sons, Inc., New York (1963)

5. Solution:

a. Results: There are two pages of output for each case of the problem: the page entitled "Input Data" simply gives the known data. The page entitled "Results" gives all the values calculated by the program.

b. Discussion of Results: The 1st case requires a total of 19 stages (including the reboiler) to perform this separation. When the entrainment is reduced to zero (2nd case), 18 stages are required. When the efficiency is increased to 1.0 (3rd case), only 14 stages are needed. In the 4th case, where L/D = 30.0, the operation approaches that of total reflux and requires only 8 stages. The 5th case uses L/D = 1.5, which is lower than the minimum reflux ratio, therefore the calculations get caught in a pinch zone.

III. EDUCATIONAL ASPECTS

1. Description of Past Usage: This problem has been assigned in a course on the design of separation processes taught in the senior year.

2. Concepts Demonstrated: The student is required to write a computer program which will perform the stage-to-stage calculations of a multistage distillation column. Such calculations, which had been previously performed by the student with the use of the McCabe-Thiele diagram, can now be programmed by him on a digital computer so that he can examine many different cases. By varying the entrainment, plate efficiency and reflux ratio, he demonstrates to himself the effect of these variables on the size of the column and the separation obtained. The values for L/D of 30.0 and 1.5 (see problem statement) were chosen so as to demonstrate explicitly the concepts of total reflux and minimum reflux, respectively. The student is not forwarned that L/D = 1.5 will result in a pinch point, he finds that out when his program indicates that a very large number of stages is required.

This type of a problem bridges the gap between the McCabe-Thiele method which is taught early in the course and the multicomponent distillation methods which are taught later on in the same course. In addition, this problem utilizes the Newton-Raphson technique for finding the correct root of the equation which relates the distribution coefficients to temperature.

3. Evaluation of Usage: The student is given the freedom to construct his own solution algorithm. It is recommended to him to break down his program into subroutines where repetitive calculations are involved (i.e. separate the equilibrium calculations into a sub-routine which will be called for each dew point or bubble point calculation).

The time spent on this problem is difficult to estimate. The instructor can describe the problem and give to the students some hints on programming in one or two 50-minute periods. The students should be allowed 2-3 weeks for completing their solutions. It is expected that each student will devote approximately 20 hours in programming the problem, debugging the program and writing the report. The total computer time (including debugging) consumed on an IBM 1130 is estimated at about 5-10 minutes per student.

The feedback obtained from the students indicated that this problem accomplished its objectives in demonstrating to the student the use of computers in multistage separations. In addition, a lot of students, especially those who had not written many computer programs in the past, found the programming aspect very challenging.

IV. PROGRAM SUMMARY SHEET

V. PROGRAM DESCRIPTION

The program consists of the main program and one subroutine. The functions of the main program are: a) to read in the known values of feed and product compositions, feed rate, feed thermal condition, initial temperature guess, efficiency, entrainment, reflux ratio and the constants for the equilibrium relations, b) to perform the overall balance calculations and the stage-to-stage calculations, and c) to call subroutine EQUIL which performs the feed flash calculation and the bubble-point calculations.

This program contains only one COMMON statement which appears in the main program and the subroutine as follows:

```
COMMON/ONE/A(2), B(2), C(2), ZF(2), QF
```

The information included in this statement are the constants (A, B & C) for the equilibrium relations, the feed composition (ZF) and the thermal condition of the feed (QF).

This program was initially written and operated on an IBM 7094 computer. It has since been modified for the IBM 360. The results shown here are those obtained using an IBM 360. The students seem to prefer to write their programs for the solution of this problem on an IBM 1130 computer which is more accessible to them and which has a faster turnaround time.

Main Program: This performs all the input and output. In addition it performs all the material balance calculations which are described in the Problem Formulation. The following are the input variables of the program given in the order in which they are read by the program:

ZF(1) = Propane mole fraction in feed
ZF(2) = N-butane mole fraction in feed
XW(1) = Propane mole fraction in bottoms
XW(2) = N-butane mole fraction in bottoms
XD(1) = Propane mole fraction in distillate
XD(2) = N-butane mole fraction in distillate
F = Feed flow rate, moles/hour
QF = Thermal condition of feed
T = Initial temperature guess for flash calculation (°F)
EFE = Murphree vapor efficiency
EE = Entrainment
ELOD = External reflux ratio (L/D)

A(1), B(1), C(1) = Constants for the equation which calculates the distribution coefficients for propane

A(2), B(2), C(2) = Constants for n-butane.

Data Input: The format to be used for the data input is as follows:

Card	Variables	Format
1st	ZF(1), ZF(2)	2F10.0
2nd	XW(1), XW(2)	2F10.0
3rd	XD(1), XD(2)	2F10.0
4th	F, QF, T	3F10.0
5th	EFE, EE, ELOD	3F10.0
6th	A(1), B(1), C(1)	3F10.0
7th	A(2), B(2), C(2)	3F10.0

Output: First, the program prints out all the data input. Then it writes out all the results of the calculations: flow rates, feed flash calculation and stage-to-stage calculations. The program will print "Iteration limit exceeded" and skip to next case, if it fails to converge on a bubble point temperature within forty iterations. The program will print "Calculations may be approaching pinch zone" if it detects that the temperature of succeeding stages does not change by more than 0.05°F.

Subroutine EQUIL: This subroutine performs the equilibrium calculations of the problem. When it is called for the first time, it calculates the flash temperature of the feed and the composition of the vapor and liquid portions of the flashed feed. Later on, it is repeatedly called to perform bubble-point calculations for all the stages.

The argument list for this subroutine includes the following variables:

N = Number of components in mixture
MI = 0 for feed flash calculation
1 for stage bubble-point calculation
K = The number corresponding to the row location in matrices X and Y
X = The matrix containing liquid compositions of stages
Y = The matrix containing vapor compositions of stages
T = Temperature, °F
ITER = Number of iterations taken to arrive at temperature.

This subroutine does not have any data input or output.

VI. PROGRAM LISTING

```
C     CONTINUOUS MULTISTAGE BINARY DISTILLATION.
C*****
C     MAIN PROGRAM
C*****
      DIMENSION XW(2), XD(2), X(100,2), Y(100,2), YE(100,2), YF(2),
     1  XF(2)
      DATA IN,IO/5,6/
      COMMON/ONE/A(2), B(2), C(2), ZF(2), QF
      NCASE=0
    1 READ(IN,101,END=47) (ZF(I),I=1,2)
      NCASE=NCASE+1
      READ(IN,101) (XW(I),I=1,2)
      READ(IN,101) (XD(I),I=1,2)
      READ(IN,102) F,QF,T
      READ(IN,102) EFE,EE,ELOD
      READ(IN,102) (A(I), B(I), C(I), I=1,2)
      WRITE(IO,110) NCASE
      WRITE(IO,111) ZF(1), ZF(2), XD(1), XD(2), XW(1), XW(2)
      WRITE(IO,112) F,QF,T,EFE,EE,ELOD
      WRITE(IO,113) A(1), B(1), C(1), A(2), B(2), C(2)
C     EXTERNAL MATERIAL BALANCES
      D=F*(ZF(1)-XW(1))/(XD(1)-XW(1))
      W=F-D
      EL=D*ELOD
      EV=EL+D
      SL=F*QF+EL
      SV=(QF-1.0)*F + EV
      WRITE(IO,110) NCASE
      WRITE(IO,114) D,W,EL,EV,SL,SV
C     PERFORM FLASH CALCULATION FOR FEED
      K=99
      CALL EQUIL(2, 0, K, X, Y, T, ITER)
      YF(1)=Y(99,1)
      XF(1)=X(99,1)
      TF=T                                                              MAIN 310
      WRITE(IO,115) Y(K,1), X(K,1), T, Y(K,2),X(K,2)                    MAIN 320
C     CALCULATE REBOILER BUBBLE POINT                                   MAIN 330
      K=1                                                               MAIN 340
      X(K,2)=XW(2)                                                      MAIN 350
      X(K,1)=XW(1)                                                      MAIN 360
      CALL EQUIL(2, 1, K, X, YE,T, ITER)                                MAIN 370
      Y(K,1)=YE(K,1)                                                    MAIN 380
      Y(K,2)=YE(K,2)                                                    MAIN 390
      WRITE(IO,116)                                                     MAIN 400
      WRITE(IO,117) K,Y(K,1), X(K,1), T, Y(K,2), X(K,2)                 MAIN 410
      IF(ITER.GT.40) GO TO 90                                           MAIN 420
C     BALANCE AROUND REBOILER                                           MAIN 430
      X(K+1,1)=(SV*Y(K,1) + W*XW(1))/SL                                 MAIN 440
      X(K+1,2)=1.0-X(K+1,1)                                             MAIN 450
C     CHECKS STAGE TEMPERATURE TO LOCATE FEED STAGE                     MAIN 460
   10 IF(T.LE.TF) GO TO 22                                              MAIN 470
C     STRIPPING SECTION CALCULATIONS                                    MAIN 480
      K=K+1                                                             MAIN 490
      TT=T                                                              MAIN 500
      CALL EQUIL(2, 1, K, X, YE,T, ITER)                                MAIN 510
      Y(K,1)=EFE*(YE(K,1)-Y(K-1,1))+Y(K-1,1)                            MAIN 520
      Y(K,2)=1.0-Y(K,1)                                                 MAIN 530
      WRITE(IO,117) K,Y(K,1), X(K,1), T, Y(K,2), X(K,2)                 MAIN 540
      IF(ITER.GT.40) GO TO 90                                           MAIN 550
      DT=ABS(TT-T)                                                      MAIN 560
      IF(DT.LE.0.05) GO TO 100                                          MAIN 570
      IF(K.GE.100) GO TO 100                                            MAIN 580
      X(K+1,1)=(SV*Y(K,1)+EE*SV*X(K,1)+W*XW(1))/(SL+EE*SV)              MAIN 590
      X(K+1,2)=1.0-X(K+1,1)                                             MAIN 600
      GO TO 10                                                          MAIN 610
   22 WRITE(IO,118) K                                                   MAIN 620
C     BALANCE ABOVE FEED STAGE.  INCLUDES THE VAPOR PORTION OF THE FEED MAIN 630
   23 X(K+1,1)=(SV*Y(K,1) + EE*SV*X(K,1) + (1.0-QF)*F*YF(1) - D*XD(1))/ MAIN 640
     1 (EL + EE*SV)                                                     MAIN 650
```

```
      X(K+1,2)=1.0-X(K+1,1)                                              MAIN 660
      K=K+1                                                              MAIN 670
      CALL EQUIL(2, 1, K, X, YE,T, ITER)                                 MAIN 680
      Y(K,1)=EFE*(YE(K,1)-Y(K-1,1))+Y(K-1,1)                             MAIN 690
      Y(K,2)=1.0-Y(K,1)                                                  MAIN 700
      WRITE(IO,117) K,Y(K,1), X(K,1), T, Y(K,2), X(K,2)                  MAIN 710
      IF(ITER.GT.40) GO TO 90                                            MAIN 720
C     BALANCE IN ENRICHING SECTION                                       MAIN 730
   30 X(K+1,1)=(EV*Y(K,1)+EE*EV*X(K,1)-D*XD(1))/(EL+EE*EV)               MAIN 740
      X(K+1,2)=1.0-X(K+1,1)                                              MAIN 750
      K=K+1                                                              MAIN 760
      TT=T                                                               MAIN 770
      CALL EQUIL(2, 1, K, X, YE,T, ITER)                                 MAIN 780
      Y(K,1)=EFE*(YE(K,1)-Y(K-1,1))+Y(K-1,1)                             MAIN 790
      Y(K,2)=1.0-Y(K,1)                                                  MAIN 800
      WRITE(IO,117) K,Y(K,1), X(K,1), T, Y(K,2), X(K,2)                  MAIN 810
      IF(ITER.GT.40) GO TO 90                                            MAIN 820
      DT=ABS(TT-T)                                                       MAIN 830
      IF(DT.LE.0.05) GO TO 100                                           MAIN 840
      IF(K.GE.100) GO TO 100                                             MAIN 850
      IF(Y(K,1).LT.XD(1)) GO TO 30                                       MAIN 860
      GO TO 95                                                           MAIN 870
   90 WRITE(IO,119)                                                      MAIN 880
   95 CONTINUE                                                           MAIN 890
      GO TO 1                                                            MAIN 900
  100 WRITE(IO,120)                                                      MAIN 910
      GO TO 1                                                            MAIN 920
   47 CONTINUE                                                           MAIN 930
  101 FORMAT(2F10.0)                                                     MAIN 940
  102 FORMAT(3F10.0)                                                     MAIN 950
  110 FORMAT(1H1, 16X, 5H CASE, I2)                                      MAIN 955
  111 FORMAT(11H INPUT DATA , //, 25X, 19H PROPANE   N-BUTANE  ,/,       MAIN 960
     123H FEED COMPOSITION        ,2F9.3,/,23H DISTILLATE COMPOSITION  , MAIN 970
     22F9.3,/, 23H BOTTOMS COMPOSITION        ,2F9.3,/)                  MAIN 980
  112 FORMAT(25H FEED RATE(F, MOLES/HR)=  ,F6.2,/,18H FEED QUALITY(QF)=,MAIN 990
     1 F6.2,/, 31H INITIAL TEMPERATURE GUESS(T)= , F6.2,/, 33H MURPHREE MAIN1000
     2VAPOR EFFICIENCY(EFE)= ,F6.2,/, 18H ENTRAINMENT(EE)= ,F6.2,/,     MAIN1010
     3 14H L/D (ELOD) = ,F6.2)                                          MAIN1020
  113 FORMAT(10H CONSTANTS  ,5X,2H A, 10X, 2H B, 10X, 2H C,/,           MAIN1030
     1 10H  PROPANE , F10.3,2F12.5,/,10H  N-BUTANE ,F10.3,2F12.5)       MAIN1040
  114 FORMAT(8H RESULTS ,//,34H CALCULATED FLOW RATES(MOLES/HR):  ,/,   MAIN1050
     114H  DISTILLATE= , F6.1,/, 11H  BOTTOMS= ,F6.1,/,28H  LIQUID(ENRICMAIN1060
     2HING SECTION)= ,F6.1,/,28H  VAPOR (ENRICHING SECTION)= ,F6.1,/,28HMAIN1070
     3  LIQUID(STRIPPING SECTION)= ,F6.1,/,28H  VAPOR (STRIPPING SECTIONMAIN1080
     4)= ,F6.1)                                                         MAIN1090
  115 FORMAT( / ,57H FLASH CALCULATION:       VAPOR    LIQUID    TEMPERAMAIN1100
     1TURE  ,/, 5X, 8H PROPANE , 11X, 2F8.4, 7X, F7.2,/, 5X, 9H N-BUTANEMAIN1110
     2 , 10X, 2F8.4)                                                    MAIN1120
  116 FORMAT(/ ,  29H STAGE-TO-STAGE CALCULATIONS: ,/, 15X, 44H STAGE NOMAIN1130
     1.  VAPOR   LIQUID    TEMPERATURE    )                             MAIN1140
  117 FORMAT(5X, 8H PROPANE ,4X, I4, 3X, 2F8.4, 7X, F7.2,/,5X,          MAIN1150
     2 9H N-BUTANE , 10X, 2F8.4)                                        MAIN1160
  118 FORMAT(47H CROSSING TO ENRICHING SECTION ABOVE STAGE NO.  ,I3)    MAIN1170
  119 FORMAT(////,26H ITERATION LIMIT EXCEEDED )                        MAIN1180
  120 FORMAT(44H CALCULATIONS MAY BE APPROACHING PINCH ZONE   )         MAIN1190
      END                                                               MAIN1200
      SUBROUTINE EQUIL(N,MI,K,X,Y,T,ITER)
C*****
C     SUBROUTINE EQUIL
C*****
C     PURPOSE
C*****
C     PERFORMS FLASH CALCULATION AND STAGE BUBBLE-POINT CALCULATIONS
C*****
      DIMENSION X(100,2), Y(100,2), AK(2), TAN(2), DFT(2), FT(2)
      COMMON/ONE/A(2), B(2), C(2), ZF(2), QF
C     CONVERTS TEMPERATURE TO ABSOLUTE
      TA=T+459.6
C     INITIALIZATION
      ITER=0
    1 JAZ=0
      SUMY=0.0
      SUMT=0.0
C     CALCULATES VALUES OF DISTRIBUTION COEFFICIENTS
      DO 10 I=1,N
      TERM=A(I)/TA + B(I) + C(I)*TA
      AK(I)=EXP(TERM)
      IF(MI-1) 2,3,3
C     FEED FLASH CALCULATION
    2 Y(K,I)=ZF(I)/(1.0+QF*(1.0/AK(I)-1.0))
      X(K,I)=Y(K,I)/AK(I)
      GO TO 4
C     SUMMATION OF Y
    3 Y(K,I)=AK(I)*X(K,I)
    4 SUMY=SUMY+Y(K,I)
   10 CONTINUE
      ITER=ITER+1
C     CHECKS FOR CONVERGENCE
      IF(ABS(SUMY-1.0).LT.0.0001) RETURN
      IF(ITER.GT.40) RETURN
      DO 20 J=1,N
C     CORRECTS VALUES OF Y
      Y(K,J)=Y(K,J)/SUMY
C     RECALCULATES DISTRIBUTION COEFFICIENTS
      AK(J)=Y(K,J)/X(K,J)
C     RECALCULATES TEMPERATURE USING THE NEWTON-RAPHSON METHOD
      FT(J)=A(J) + (B(J)-ALOG(AK(J)))*TA + C(J)*TA*TA
      DFT(J)=B(J)-ALOG(AK(J)) + 2.0*C(J)*TA
      TAN(J)=TA-(FT(J)/DFT(J))
      IF(ABS(TAN(J)-TA).GT.0.01) JAZ=1
      SUMT=SUMT+TAN(J)
   20 CONTINUE
      IF(JAZ.EQ.0) GO TO 30
      W=N
      TA=SUMT/W
      T=TA-459.6
      GO TO 1
   30 RETURN
      END
```

```
                         CASE 1
INPUT DATA

                                  PROPANE    N-BUTANE
FEED COMPOSITION                   0.500      0.500
DISTILLATE COMPOSITION             0.900      0.100
BOTTOMS COMPOSITION                0.100      0.900

FEED RATE(F. MOLES/HR)= 100.00
FEED QUALITY(QF)=   0.20
INITIAL TEMPERATURE GUESS(T)= 160.00
MURPHREE VAPOR EFFICIENCY(EFE)=    0.70
ENTRAINMENT(EE)=    0.10
L/D (ELOD) =    2.00
CONSTANTS          A             B              C
 PROPANE   -3987.933      8.63131      -0.00290
 N-BUTANE -4760.750       8.50187      -0.00206
```

```
                    CASE 1
RESULTS

CALCULATED FLOW RATES(MOLES/HR):
 DISTILLATE=    50.0
 BOTTOMS=    50.0
 LIQUID(ENRICHING SECTION)= 100.0
 VAPOR (ENRICHING SECTION)= 150.0
 LIQUID(STRIPPING SECTION)= 120.0
 VAPOR (STRIPPING SECTION)=  70.0

FLASH CALCULATION:          VAPOR    LIQUID      TEMPERATURE
      PROPANE               0.5403   0.3390         169.27
      N-BUTANE              0.4596   0.6614

STAGE-TO-STAGE CALCULATIONS:
                   STAGE NO.  VAPOR    LIQUID      TEMPERATURE
      PROPANE          1      0.1914   0.1000         196.34
      N-BUTANE                0.8085   0.9000
      PROPANE          2      0.2547   0.1533         190.04
      N-BUTANE                0.7453   0.8467
      PROPANE          3      0.3122   0.1882         186.00
      N-BUTANE                0.6878   0.8118
      PROPANE          4      0.3645   0.2218         182.17
      N-BUTANE                0.6355   0.7782
      PROPANE          5      0.4104   0.2525         178.73
      N-BUTANE                0.5896   0.7475
      PROPANE          6      0.4496   0.2795         175.74
      N-BUTANE                0.5504   0.7205
      PROPANE          7      0.4821   0.3026         173.22
      N-BUTANE                0.5179   0.6974
      PROPANE          8      0.5085   0.3218         171.15
      N-BUTANE                0.4915   0.6782
      PROPANE          9      0.5295   0.3374         169.48
      N-BUTANE                0.4705   0.6626
      PROPANE         10      0.5461   0.3498         168.16
      N-BUTANE                0.4539   0.6502
 CROSSING TO ENRICHING SECTION ABOVE STAGE NO.       10
      PROPANE         11      0.5620   0.3635         166.72
      N-BUTANE                0.4380   0.6365
      PROPANE         12      0.5866   0.3891         164.08
      N-BUTANE                0.4134   0.6109
      PROPANE         13      0.6201   0.4246         160.45
      N-BUTANE                0.3799   0.5754
      PROPANE         14      0.6630   0.4729         155.66
      N-BUTANE                0.3370   0.5271
      PROPANE         15      0.7143   0.5352         149.68
      N-BUTANE                0.2857   0.4648
      PROPANE         16      0.7707   0.6102         142.81
      N-BUTANE                0.2293   0.3898
      PROPANE         17      0.8272   0.6936         135.58
      N-BUTANE                0.1728   0.3064
      PROPANE         18      0.8786   0.7781         128.67
      N-BUTANE                0.1214   0.2219
      PROPANE         19      0.9216   0.8561         122.64
      N-BUTANE                0.0784   0.1439
```

```
                    CASE 2
INPUT DATA

                                PROPANE    N-BUTANE
FEED COMPOSITION                 0.500      0.500
DISTILLATE COMPOSITION           0.900      0.100
BOTTOMS COMPOSITION              0.100      0.900

FEED RATE(F, MOLES/HR)= 100.00
FEED QUALITY(QF)=  0.20
INITIAL TEMPERATURE GUESS(T)= 160.00
MURPHREE VAPOR EFFICIENCY(EFE)=    0.70
ENTRAINMENT(EE)=    0.0
L/D (ELOD) =    2.00
CONSTANTS        A             B             C
 PROPANE  -3987.933     8.63131      -0.00290
 N-BUTANE -4760.750     8.50187      -0.00206
```

```
                      CASE 2
RESULTS

CALCULATED FLOW RATES(MOLES/HR):
 DISTILLATE=    50.0
 BOTTOMS=    50.0
 LIQUID(ENRICHING SECTION)= 100.0
 VAPOR (ENRICHING SECTION)= 150.0
 LIQUID(STRIPPING SECTION)= 120.0
 VAPOR (STRIPPING SECTION)=  70.0

FLASH CALCULATION:          VAPOR     LIQUID      TEMPERATURE
     PROPANE                0.5403   0.3390         169.27
     N-BUTANE               0.4596   0.6614

STAGE-TO-STAGE CALCULATIONS:
                   STAGE NO.  VAPOR    LIQUID      TEMPERATURE
     PROPANE           1    0.1914   0.1000         196.34
     N-BUTANE               0.8085   0.9000
     PROPANE           2    0.2547   0.1533         190.04
     N-BUTANE               0.7453   0.8467
     PROPANE           3    0.3144   0.1902         185.77
     N-BUTANE               0.6856   0.8098
     PROPANE           4    0.3684   0.2250         181.80
     N-BUTANE               0.6316   0.7750
     PROPANE           5    0.4155   0.2565         178.28
     N-BUTANE               0.5845   0.7435
     PROPANE           6    0.4553   0.2840         175.24
     N-BUTANE               0.5447   0.7160
     PROPANE           7    0.4879   0.3072         172.72
     N-BUTANE               0.5121   0.6928
     PROPANE           8    0.5140   0.3263         170.67
     N-BUTANE               0.4860   0.6737
     PROPANE           9    0.5346   0.3415         169.04
     N-BUTANE               0.4654   0.6585
CROSSING TO ENRICHING SECTION ABOVE STAGE NO.   9
     PROPANE          10    0.5529   0.3564         167.47
     N-BUTANE               0.4471   0.6436
     PROPANE          11    0.5765   0.3794         165.07
     N-BUTANE               0.4235   0.6206
     PROPANE          12    0.6099   0.4147         161.45
     N-BUTANE               0.3901   0.5853
     PROPANE          13    0.6547   0.4649         156.44
     N-BUTANE               0.3453   0.5351
     PROPANE          14    0.7100   0.5321         149.98
     N-BUTANE               0.2900   0.4679
     PROPANE          15    0.7719   0.6150         142.38
     N-BUTANE               0.2281   0.3850
     PROPANE          16    0.8337   0.7078         134.39
     N-BUTANE               0.1663   0.2922
     PROPANE          17    0.8889   0.8005         126.91
     N-BUTANE               0.1111   0.1995
     PROPANE          18    0.9335   0.8833         120.62
     N-BUTANE               0.0665   0.1167
```

```
                      CASE 3
INPUT DATA

                                     PROPANE    N-BUTANE
FEED COMPOSITION                      0.500      0.500
DISTILLATE COMPOSITION                0.900      0.100
BOTTOMS COMPOSITION                   0.100      0.900

FEED RATE(F, MOLES/HR)= 100.00
FEED QUALITY(QF)=   0.20
INITIAL TEMPERATURE GUESS(T)= 160.00
MURPHREE VAPOR EFFICIENCY(EFE)=    1.00
ENTRAINMENT(EE)=    0.10
L/D (ELOD) =    2.00
CONSTANTS          A               B             C
 PROPANE  -3987.933        8.63131       -0.00290
 N-BUTANE -4760.750        8.50187       -0.00206
```

```
                    CASE 3
RESULTS

CALCULATED FLOW RATES(MOLES/HR):
 DISTILLATE=    50.0
 BOTTOMS=    50.0
 LIQUID(ENRICHING SECTION)= 100.0
 VAPOR (ENRICHING SECTION)= 150.0
 LIQUID(STRIPPING SECTION)= 120.0
 VAPOR (STRIPPING SECTION)=  70.0

FLASH CALCULATION:            VAPOR     LIQUID     TEMPERATURE
     PROPANE                  0.5403    0.3390        169.27
     N-BUTANE                 0.4596    0.6614

STAGE-TO-STAGE CALCULATIONS:
                   STAGE NO.  VAPOR     LIQUID     TEMPERATURE
     PROPANE           1      0.1914    0.1000        196.34
     N-BUTANE                 0.8085    0.9000
     PROPANE           2      0.2818    0.1533        190.04
     N-BUTANE                 0.7182    0.8467
     PROPANE           3      0.3594    0.2032        184.29
     N-BUTANE                 0.6406    0.7968
     PROPANE           4      0.4248    0.2487        179.15
     N-BUTANE                 0.5752    0.7513
     PROPANE           5      0.4765    0.2872        174.89
     N-BUTANE                 0.5235    0.7128
     PROPANE           6      0.5150    0.3178        171.57
     N-BUTANE                 0.4850    0.6822
     PROPANE           7      0.5425    0.3407        169.13
     N-BUTANE                 0.4575    0.6593
CROSSING TO ENRICHING SECTION ABOVE STAGE NO.  7
     PROPANE           8      0.5655    0.3606        167.03
     N-BUTANE                 0.4345    0.6394
     PROPANE           9      0.6017    0.3933        163.63
     N-BUTANE                 0.3983    0.6067
     PROPANE          10      0.6546    0.4448        158.42
     N-BUTANE                 0.3454    0.5552
     PROPANE          11      0.7240    0.5205        151.06
     N-BUTANE                 0.2760    0.4795
     PROPANE          12      0.8026    0.6209        141.86
     N-BUTANE                 0.1974    0.3791
     PROPANE          13      0.8773    0.7366        132.02
     N-BUTANE                 0.1227    0.2634
     PROPANE          14      0.9367    0.8491        123.16
     N-BUTANE                 0.0633    0.1509
```

```
                         CASE 4
INPUT DATA

                                 PROPANE    N-BUTANE
FEED COMPOSITION                  0.500      0.500
DISTILLATE COMPOSITION            0.900      0.100
BOTTOMS COMPOSITION               0.100      0.900

FEED RATE(F, MOLES/HR)= 100.00
FEED QUALITY(QF)=   0.20
INITIAL TEMPERATURE GUESS(T)= 160.00
MURPHREE VAPOR EFFICIENCY(EFE)=    0.70
ENTRAINMENT(EE)=    0.10
L/D (ELOD) =   30.00
CONSTANTS          A              B              C
 PROPANE  -3987.933       8.63131       -0.00290
 N-BUTANE -4760.750       8.50187       -0.00206
```

```
                 CASE 4
RESULTS

CALCULATED FLOW RATES(MOLES/HR):
 DISTILLATE=    50.0
 BUTTOMS=    50.0
 LIQUID(ENRICHING SECTION)=1500.0
 VAPOR (ENRICHING SECTION)=1550.0
 LIQUID(STRIPPING SECTION)=1520.0
 VAPOR (STRIPPING SECTION)=1470.0

FLASH CALCULATION:              VAPOR    LIQUID      TEMPERATURE
     PROPANE                    0.5403   0.3390         169.27
     N-BUTANE                   0.4596   0.6614

STAGE-TO-STAGE CALCULATIONS:
                       STAGE NO.  VAPOR    LIQUID      TEMPERATURE
     PROPANE             1      0.1914   0.1000         196.34
     N-BUTANE                   0.8085   0.9000
     PROPANE             2      0.2934   0.1884         185.97
     N-BUTANE                   0.7066   0.8116
     PROPANE             3      0.4134   0.2784         175.86
     N-BUTANE                   0.5866   0.7216
     PROPANE             4      0.5443   0.3921         163.75
     N-BUTANE                   0.4557   0.6079
CROSSING TO ENRICHING SECTION ABOVE STAGE NO.   4
     PROPANE             5      0.6696   0.5197         151.14
     N-BUTANE                   0.3304   0.4803
     PROPANE             6      0.7762   0.6486         139.44
     N-BUTANE                   0.2238   0.3514
     PROPANE             7      0.8566   0.7605         130.08
     N-BUTANE                   0.1434   0.2395
     PROPANE             8      0.9117   0.8463         123.39
     N-BUTANE                   0.0883   0.1537
```

```
                     CASE 5
INPUT DATA

                                 PROPANE    N-BUTANE
FEED COMPOSITION                  0.500      0.500
DISTILLATE COMPOSITION            0.900      0.100
BOTTOMS COMPOSITION               0.100      0.900

FEED RATE(F, MOLES/HR)= 100.00
FEED QUALITY(QF)=  0.20
 INITIAL TEMPERATURE GUESS(T)= 160.00
MURPHREE VAPOR EFFICIENCY(EFE)=    0.70
ENTRAINMENT(EE)=    0.10
L/D (ELOD) =     1.50
CONSTANTS        A              B            C
 PROPANE  -3987.933      8.63131     -0.00290
 N-BUTANE -4760.750      8.50187     -0.00206
```

```
                    CASE 5
RESULTS

CALCULATED FLOW RATES(MOLES/HR):
 DISTILLATE=    50.0
 BOTTOMS=    50.0
 LIQUID(ENRICHING SECTION)=  75.0
 VAPOR (ENRICHING SECTION)= 125.0
 LIQUID(STRIPPING SECTION)=  95.0
 VAPOR (STRIPPING SECTION)=  45.0

FLASH CALCULATION:          VAPOR    LIQUID     TEMPERATURE
     PROPANE                0.5403   0.3390        169.27
     N-BUTANE               0.4596   0.6614

STAGE-TO-STAGE CALCULATIONS:
                  STAGE NO.  VAPOR    LIQUID     TEMPERATURE
     PROPANE          1     0.1914   0.1000        196.34
     N-BUTANE               0.8085   0.9000
     PROPANE          2     0.2432   0.1433        191.21
     N-BUTANE               0.7568   0.8567
     PROPANE          3     0.2853   0.1667        188.48
     N-BUTANE               0.7147   0.8333
     PROPANE          4     0.3199   0.1868        186.16
     N-BUTANE               0.6801   0.8132
     PROPANE          5     0.3478   0.2034        184.28
     N-BUTANE               0.6522   0.7966
     PROPANE          6     0.3700   0.2167        182.75
     N-BUTANE               0.6300   0.7833
     PROPANE          7     0.3874   0.2274        181.54
     N-BUTANE               0.6126   0.7726
     PROPANE          8     0.4010   0.2358        180.60
     N-BUTANE               0.5990   0.7642
     PROPANE          9     0.4115   0.2423        179.87
     N-BUTANE               0.5885   0.7577
     PROPANE         10     0.4195   0.2473        179.30
     N-BUTANE               0.5805   0.7527
     PROPANE         11     0.4256   0.2512        178.87
     N-BUTANE               0.5744   0.7488
     PROPANE         12     0.4303   0.2541        178.54
     N-BUTANE               0.5697   0.7459
     PROPANE         13     0.4339   0.2564        178.29
     N-BUTANE               0.5661   0.7436
     PROPANE         14     0.4366   0.2581        178.09
     N-BUTANE               0.5634   0.7419
     PROPANE         15     0.4386   0.2594        177.95
     N-BUTANE               0.5614   0.7406
     PROPANE         16     0.4401   0.2603        177.85
     N-BUTANE               0.5599   0.7397
     PROPANE         17     0.4413   0.2611        177.76
     N-BUTANE               0.5587   0.7389
     PROPANE         18     0.4422   0.2616        177.70
     N-BUTANE               0.5578   0.7384
     PROPANE         19     0.4429   0.2621        177.66
     N-BUTANE               0.5571   0.7379
CALCULATIONS MAY BE APPROACHING PINCH ZONE
```

I. PROBLEM IDENTIFICATION

1. Title: Batch Distillation of Moonshine
2. Author: W. L. Luyben
3. Affiliation: Lehigh University

II. TECHNICAL DESCRIPTION

1. Problem Statement: To prepare for an up-coming confrontation with the Hatfields, Grandpa McCoy is planning to distill a batch of his corn whiskey.

He fills the kettle with a pseudo-binary 50/50 molar mixture of ethanol and water (relative volatility is approximately 2.0). He then builds a hickory-wood fire under the kettle and adds fresh logs at a rate that maintains a constant boilup of 10 moles/hour of vapor.

Above the kettle is a ten-tray distillation column. Tray efficiency is 100%. Equimolal overflow can be assumed. Holdup of material on the trays is so small that it can be neglected.

Vapor leaving the top of the column is condensed in an old automobile radiator. Liquid holdup in the condenser and reflux piping is negligible. Liquid reflux at its bubble point is returned to the top plate at a rate of 7.5 moles/hour, leaving 2.5 moles/hour of McCoy's "Liquid Lightning" product for jug storage.

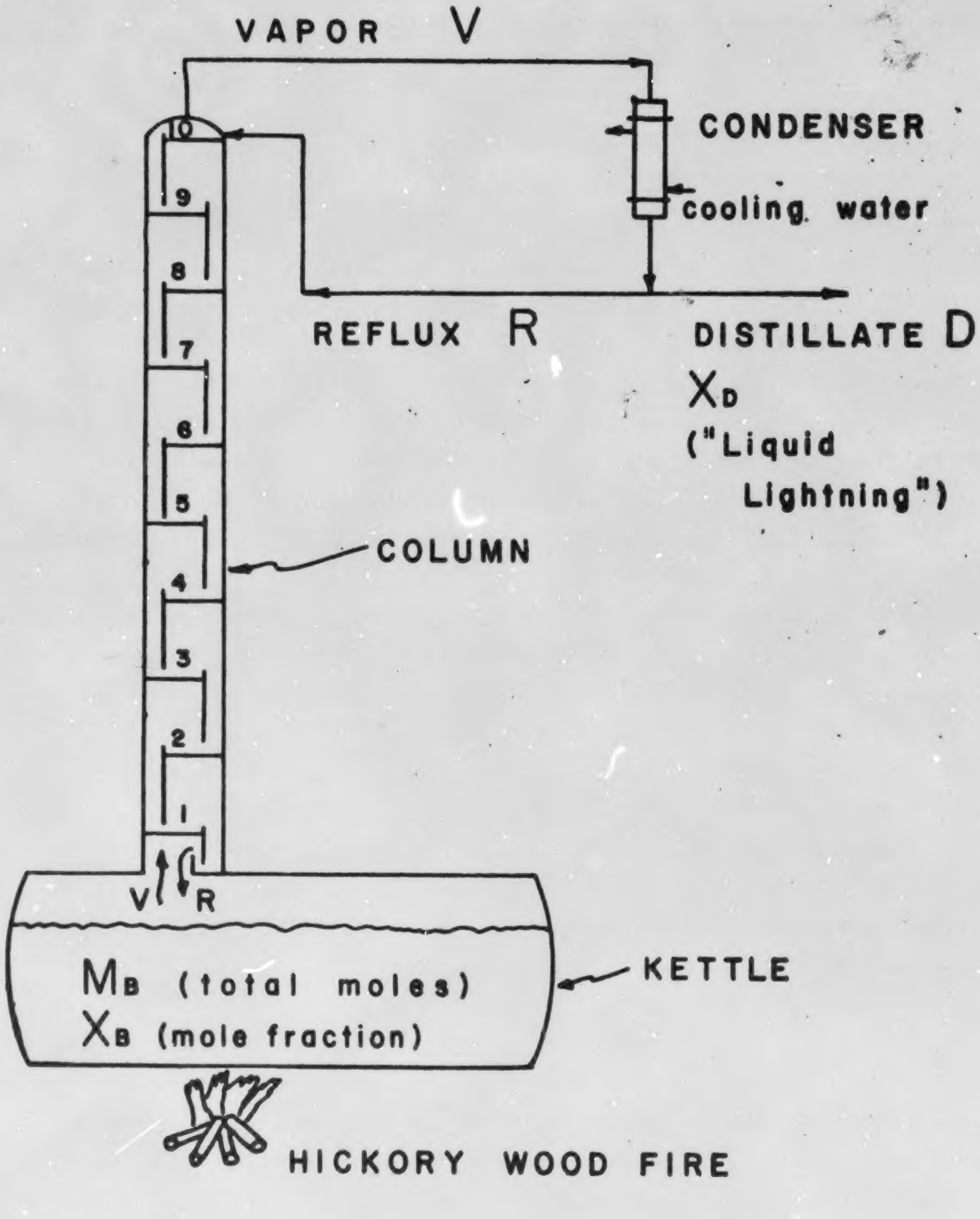
The system is sketched in Figure 1.

Determine how distillate composition $X_{D(t)}$ and kettle composition $X_{B(t)}$ vary dynamically with time over the course of a 24 hour batch.

2. Problem Formulation and Technical Analysis:

Batch distillation columns are still used in many chemical plants because of their advantages in some systems (eg. many products from a single column).

Since batch distillation is inherently dynamic in nature, differential equations must be used to describe the variations in compositions and still-pot holdup with time.


VAPOR V
10
9
8
7
6
5
4
3
2
1
CONDENSER
cooling water
REFLUX R
DISTILLATE D
XD
("Liquid Lightning")
COLUMN
V
R
MB (total moles)
XB (mole fraction)
KETTLE
HICKORY WOOD FIRE

If the holdup of material on the trays and in the condenser and reflux piping is negligible, the material in the kettle represents the only capacitance in the system. Therefore two ordinary differential equations are required.

$$\frac{dM_B}{dt} = -D \tag{1}$$

$$\frac{d\,(M_B X_B)}{dt} = -D\ X_D \tag{2}$$

Ordinary differential equations result because we have assumed that the material in the kettle is perfectly mixed, leaving time t as the only independent variable.

Equation (1) can be integrated analytically in this problem since D is a constant. To integrate Equation (2) we need to know the relationship between X_D and X_B. In theory, an analytical relationship, the "Smoker" equation, could be used (Ref. 2) since we have assumed constant relative volatility and equimolal overflow.

In practice, however, it is much easier to integrate Equation (2) numerically, using iterative tray-to-tray calculations at each instant in time to find what X_D must be for the X_B that exits at that instant in time.

3. Method of Solution: The trial-and-error technique used in the program consists of the following steps:

(a) At some time t, the values of M_B and X_B are known. Likewise V, R and D are known (and constant in this problem). The composition above the vapor leaving the kettle Y_B is calculated from the relative volatility α.

$$Y_B = \frac{\alpha\ X_B}{1 + (\alpha - 1)\ X_B} \tag{3}$$

(b) A value of the liquid composition on the first tray X_1 is guessed. This X_1 must obviously always be greater than the kettle composition X_B.

(c) The vapor composition above the first tray is calculated from the relative volatility α.

$$Y_1 = \frac{\alpha X_1}{1 + (\alpha-1) X_1} \tag{4}$$

(d) The liquid composition on the second tray X_2 is calculated from a component balance around the Tray 1. Liquid holdup on Tray 1 is assumed negligible so this component balance is simply an algebraic equation.

$$\text{In} - \text{Out} = \text{Accumulation} = 0$$

$$(R X_2 + V Y_B) - (R X_1 + V Y_1) = 0 \tag{5}$$

$$X_2 = X_1 + (Y_1 - Y_B) V/R \tag{6}$$

(e) The vapor composition Y_2 is calculated from the relative volatility.

(f) The liquid and vapor compositions are calculated by stepping up the ten-tray column alternately using the "operating line" equation and the equilibrium equation

$$X_{n+1} = X_n + (Y_n - Y_{n-1}) V/R \tag{7}$$

$$Y_n = \frac{\alpha X_n}{1 + (\alpha-1) X_n} \tag{8}$$

(g) At the top (tenth) tray, a reflux composition (X_{11} or X_D) is calculated from Equation (7), and a Tray 10 vapor composition Y_{10} is calculated from Equation (8).

(h) If the correct value of X_1 has been used, the calculated Y_{10} must equal the calculated X_D. Graphically this means that the ten steps up the column plus the reboiler must end by intersecting the 45-degree line on a McCabe-Thiele diagram.

(i) If the X_D calculated does not equal the Y_{10} calculated, a new guess of X_1 must be made. A simple "Interval Halving" convergence technique is used in the program. If X_D is greater than Y_{10}, the guessed value of X_1 is too high. So X_1 is reduced by a small increment DX1, which is made progressively smaller (halved) at each iteration.

The simpliest numerical integration technique for solving Equations (1) and (2) is a first-order "Euler" algorithm (Ref. 1):

$$(M_B)_{t+\Delta t} = (M_B)_t + \left[\frac{dM_B}{dt}\right]_t \Delta t \tag{9}$$

$$(M_B X_B)_{t+\Delta t} = (M_B X_B)_t + \left[\frac{d(M_B X_B)}{dt}\right]_t \Delta t \tag{10}$$

We are predicting what the values of (M_B) and $(M_B X_B)$ will be Δt hours later in time from the current values and the rates at which they are changing (their derivatives).

4. References:

(1) Luyben, W. L., "Process Modeling, Simulation and Control for Chemical Engineers", McGraw-Hill, 1973

(2) Smith, B. D., "Design of Equilibrium Stage Processes", McGraw-Hill, 1963

5. Solution:

(a) Results: Calculated values of various compositions throughout the column and the amount of material left in the kettle are printed as functions of time.

(b) Discussion of Results: The purity of the overhead X_D starts out quite high. But after ten hours the purity begins to drop rapidly. If 70 mole % were the minimum acceptable purity, "Liquid Lightning" could only be jugged for 17 hours. The total production would be 42.5 moles or about 275 one-gallon jugs.

III. EDUCATIONAL ASPECTS

1. Description of Past Usage: Senior students in a mathematical modeling and simulation course have been assigned this problem as a one-week homework project after they have been exposed to the concepts of iterative convergence methods and numerical integration of ordinary differential equations.

2. Concepts Demonstrated: (a) A dynamic, time-varying process; (b) trial-and-error solution of implicit equations; (c) numerical integration of ordinary differential equations.

3. Evaluation of Usage: The numerical integration is more easily grasped and programmed by the students than the iterative convergence. The problem is quite effective in giving them an appreciation for dynamic processes.

```
      PROGRAM BATCH(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT)
C
C
C     BATCH DISTILLATION OF MOONSHINE
C
C      AUTHOR
C           W. L. LUYBEN
C           LEHIGH UNIVERSITY
C           BETHLEHEM, PA.
C
C
C      PURPOSE
C
C      NUMERICALLY INTEGRATES THE ORDINARY DIFFERENTIAL EQUATIONS
C           DESCRIBING A BINARY BATCH DISTILLATION COLUMN WITH
C           NEGLIGIBLE TRAY AND CONDENSER HOLDUP.
C
C
C      IMPORTANT VARIABLES
C
C
C      X(N)    =  LIQUID COMPOSITION ON N-TH TRAY (MOLE FRACTION)
C
C      Y(N)    =  VAPOR COMPOSITION ABOVE N-TH TRAY (MOLE FRACTION)
C
C      XB      =  COMPOSITION OF LIQUID IN KETTLE AT BASE OF
C                   DISTILLATION COLUMN (MOLE FRACTION)
C
C      YB      =  COMPOSITION OF VAPOR LEAVING KETTLE (MOLE FRACTION)
C
C      XD      =  COMPOSITION OF OVERHEAD DISTILLATE PRODUCT LEAVING
C                   CONDENSER (MOLE FRACTION)
C
C      MB      =  HOLDUP OF LIQUID IN KETTLE (MOLES)
C
C      MBXB    =  HOLDUP OF MORE VOLATILE COMPONENT IN THE KETTLE
C                   (MOLES OF ETHANOL)
C
C      DMB     =  DERIVATIVE OF MB - TIME RATE OF CHANGE
C
C      DMBXB   =  DERIVATIVE OF MBXB - TIME RATE OF CHANGE
C
C      ALPHA   =  RELATIVE VOLATILITY
C
C      V       =  VAPOR BOILUP RATE (MOLES/HOUR)
C
C      R       =  REFLUX FLOW RATE (MOLES/HOUR)
C
C      D       =  DISTILLATE FLOW RATE (MOLES/HOUR)
C
C      TIME    =  INDEPENDENT VARIABLE TIME (HOURS)
C
C      DELTA   =  NUMERICAL INTEGRATION TIME STEP OR INTERVAL (HOURS)
C
C      DX1     =  INCREMENT THAT IS ADDED TO OR SUBTRACTED FROM THE
C                   GUESS OF X(1) TO DRIVE XD EQUAL TO Y(NT)
C
```

```
         C       NT      =  NUMBER OF THEORETICAL STAGES IN DISTILLATION COLUMN
         C
         C       TSTOP   =  TOTAL BATCH TIME (HOURS)
         C
         C
         C       DATA  INPUT
         C
         C
         C           VARIABLES ON ONE DATA CARD =  NT,ALPHA,XB,MB,TSTOP,DELTA,V,R
         C           FORMAT =    I10.7F10.5
         C
         C
         C       OUTPUT
         C
         C
         C           1.  INPUT DATA PLAYBACK.
         C
         C           2.  TABLE OF TIME, KETTLE HOLDUP, AND COMPOSITIONS FROM
         C                   TIME = 0  TO TIME = TSTOP.
         C
         C
         C       LIMITATIONS
         C
         C           1. TOTAL NUMBER OF TRAYS NT CANNOT EXCEED 100 WITHOUT
         C                            CHANGING DIMENSION STATEMENT.
         C
         C           2. SYSTEM IS LIMITED TO BINARY,EQUIMOLAL OVERFLOW, CONSTANT
         C                            RELATIVE VOLATILITY MIXTURES.
         C
         C           3. THEORETICAL TRAYS ARE ASSUMED.
         C
         C           4. THE CONDENSER IS A TOTAL CONDENSER.  REFLUX IS RETURNED
         C                            TO THE COLUMN AS A SATURATED LIQUID.
         C
         C           5. VAPOR BOILUP AND REFLUX ARE ASSUMED CONSTANT.
         C
         C           6. HOLDUPS ON ALL TRAYS AND IN THE REFLUX PIPING AND
         C                            CONDENSER ARE ASSUMED TO BE NEGLIGIBLE.
         C
         C ******************************************************************
         C ******************************************************************
         C ******************************************************************
         C ******************************************************************
         C
         C       MAIN PROGRAM  BATCH
         C
         C ******************************************************************
         C ******************************************************************
         C ******************************************************************
         C
000003          DIMENSION X(101),Y(100)
000003          REAL MB,MBXB
000003          DATA INP,IOUT/5,6/
         C
         C ******************************************************************
         C
         C     USE FUNCTION STATEMENT FOR VAPOR LIQUID EQUILIBRIUM
         C                   (CONSTANT RELATIVE VOLATILITY)
         C
         C *********************************************************************
         C
000003         EQUIL(XX)=ALPHA*XX/(1.+(ALPHA-1.)*XX)
         C
         C *********************************************************************
         C
         C      READ INPUT DATA    -  NT,ALPHA,XB,MB,TSTOP,DELTA,V,R
         C
         C                               FORMAT(I10,7F10.5)
         C
         C *********************************************************************
         C
000013         READ(INP,10)NT,ALPHA,XB,MB,TSTOP,DELTA,V,R
000037      10 FORMAT(I10,7F10.5)
         C
         C
000037         WRITE(IOUT,15)
000043      15 FORMAT(1H1,10X,85H  NT        ALPHA     XB          MB      TSTOP
              1    DELTA     V        R              )
000043         WRITE(IOUT,20)NT,ALPHA,XB,MB,TSTOP,DELTA,V,R
000067      20 FORMAT(7X,I10,3X,7F10.5)
         C
         C *********************************************************************
         C
         C      SET UP INITIAL CONDITIONS
         C
         C *********************************************************************
         C
000067         MBXB=MB*XB
000071         D=V-R
000073         TIME=0.
000074         TPRINT=0.
000075         WRITE(IOUT,1)
000100       1 FORMAT(/,5X,75H  TIME      MB        XB        X(1)      X(5)
              1X(10)     XD                 )
         C
         C *********************************************************************
         C
         C      MAIN LOOP THROUGH COLUMN FOR DERIVATIVE EVALUATIONS
         C                 AT EACH INSTANT IN TIME.
         C
         C *********************************************************************
         C
000100     100 YB=EQUIL(XB)
000101         LOOP=0
000102         FLAG=-1.
         C
         C *********************************************************************
         C
         C    INITIAL GUESS OF X(1)
         C
         C *********************************************************************
         C
000104         X(1)=XB
         C
000105         DX1=X(1)/20.
         C
```

```
        C    CONVERGENCE LOOP FOR X(1)
        C
000110     90 Y(1)=EQUIL(X(1))
000111        LOOP=LOOP+1
000113        IF(LOOP.GT.100)GO TO 700
000116        X(2)=X(1)+(Y(1)-YB)*V/R
        C
        C ***************************************************************
        C
        C    CALCULATING UP THE COLUMN
        C
        C ***************************************************************
        C
000123        DO 95 N=2,NT
000124        Y(N)=EQUIL(X(N))
000127        X(N+1)=X(N)+(Y(N)-Y(N-1))*V/R
000134        IF(X(N+1) .GT.  Y(N)+.00001)GO TO 80
000141     95 CONTINUE
        C
        C ***************************************************************
        C
        C    TEST FOR CONVERGENCE
        C
        C ***************************************************************
        C
000143        XD=X(NT+1)
000144        IF(ABS(XD-Y(NT)) .LT. .00001) GO TO 50
000151        IF(XD-Y(NT)) 85,85,80
        C
        C      INCREASE GUESS OF X(1)
        C
000153     85 IF(FLAG.LT.0.) GO TO 81
000155        DX1=DX1/2.
000156     81 X(1)=X(1)+DX1
000160        GO TO 90
        C
        C      DECREASE GUESS OF X(1)
        C
000161     80 DX1=DX1/2.
000163        X(1)=X(1)-DX1
000164        IF(X(1).LE.XB) GO TO  81
000167        FLAG=1.
000170        GO TO 90
        C
        C
        C ***************************************************************
        C
        C      WHEN CORRECT X(1) HAS BEEN FOUND, DERIVATIVES CAN BE EVALUATED.
        C
        C ***************************************************************
        C
000171     50 DMB=-D
000172        DMBXB=-XD*D
        C
        C      CHECK FOR END OF BATCH TIME
        C
000174        IF(TIME.GT.TSTOP) STOP
        C
```

```
           C
           C *******************************************************************
           C
           C    PRINT RESULTS EVERY  HOUR
           C
           C *******************************************************************
           C
000201          IF(TIME.LT. TPRINT -.02)     GO TO 40
000205          TPRINT=TPRINT+1.
000207          WRITE(IOUT,49)TIME,MB,XB,X(1),X(5),X(10),XD
000230        49 FORMAT(1X,10F10.4)
           C
           C
           C *******************************************************************
           C *******************************************************************
           C
           C      NUMERICAL INTEGRATION ALA EULER
           C
           C *******************************************************************
           C *******************************************************************
           C
000230        40 TIME=TIME+DELTA
000232          MBXB=MBXB + DMBXB*DELTA
000234          MB=MB + DMB*DELTA
000237          XB=MBXB/MB
           C
           C *******************************************************************
           C
           C     RETURN FOR NEW DERIVATIVE EVALUATIONS
           C
           C *******************************************************************
           C
000240          GO TO 100
           C
           C    PRINT OUT IF CONVERGENCE LOOP GETS INTO TROUBLE
           C
000241       700 WRITE(IOUT,701)
000245       701 FORMAT(1X,10HX1 LOOP    )
000245          STOP
000247          END
```

```
          NT          ALPHA       XB         MB          TSTOP       DELTA       V            R
            10        2.00000      .50000 100.00000  24.00000      .05000  10.00000    7.50000

     TIME        MB            XB          X(1)         X(5)         X(10)        XD
   0.0000   100.0000        .5000       .5589        .8260        .9799        .9898
   1.0000    97.5000        .4875       .5443        .8137        .9781        .9889
   2.0000    95.0000        .4743       .5286        .7996        .9759        .9878
   3.0000    92.5000        .4604       .5119        .7833        .9733        .9864
   4.0000    90.0000        .4458       .4940        .7644        .9701        .9848
   5.0000    87.5000        .4304       .4749        .7420        .9660        .9827
   6.0000    85.0000        .4142       .4544        .7154        .9607        .9800
   7.0000    82.5000        .3971       .4326        .6835        .9538        .9763
   8.0000    80.0000        .3791       .4093        .6451        .9443        .9713
   9.0000    77.5000        .3601       .3847        .5989        .9307        .9641
  10.0000    75.0000        .3401       .3590        .5448        .9112        .9535
  11.0000    72.5000        .3192       .3327        .4843        .8829        .9378
  12.0000    70.0000        .2975       .3064        .4222        .8432        .9150
  13.0000    67.5000        .2751       .2808        .3643        .7919        .8839
  14.0000    65.0000        .2524       .2558        .3140        .7314        .8448
  15.0000    62.5000        .2296       .2316        .2714        .6650        .7988
  16.0000    60.0000        .2069       .2081        .2352        .5961        .7470
  17.0000    57.5000        .1845       .1853        .2036        .5273        .6905
  18.0000    55.0000        .1628       .1633        .1757        .4603        .6304
  19.0000    52.5000        .1420       .1422        .1507        .3965        .5678
  20.0000    50.0000        .1222       .1223        .1281        .3369        .5040
  21.0000    47.5000        .1037       .1038        .1077        .2822        .4402
  22.0000    45.0000        .0866       .0867        .0894        .2329        .3778
  23.0000    42.5000        .0712       .0712        .0731        .1891        .3180
  24.0000    40.0000        .0575       .0575        .0587        .1509        .2622
```

I. PROBLEM IDENTIFICATION

1. Title: Binary Distillation Using McCabe-Thiele Assumptions
2. Author: John D. Stevens
3. Affiliation: Iowa State University

II. TECHNICAL DESCRIPTION

1. Problem Statement: A company wishes to use an existing distillation column to produce an overhead product containing 99.5% A. The feed contains 60% A (40% B) and is 50% vapor (f = 0.5). The rectifying section contains 20 actual plates and the stripping section has 15 actual plates. The plates are 80% efficient so the column can be thought of as having 16 ideal plates in the rectifying section and 12 in the stripping section (including reboiler). The relative volatility of A is 1.95.

Write and run a general computer program to determine the reflux ratio which must be used to effect this separation. What is the bottom composition? After the correct reflux ratio has been determined print out the plate number, liquid composition, and vapor composition for the 28 ideal plates. If trial and error is used print results after each iteration.

Discussion:

The reflux ratio can be determined using the rectifying section only. Solve this phase of the problem before going on to the stripping section. Use the trial and error method discussed in class to get the composition x_{16} to converge to the value of x at the intersection of the operating line and feed line. These should be within 0.001 of one another. This can be done by choosing a value for R_D and then, beginning at x_D, step off 16 plates. If the value of x_{16} and $x_{intersection}$ don't match, guess a new value for R_D and repeat the process.

For the stripping section guess x_B (equal to x_1) and step up the column. The value of x_{13} should match $x_{intersection}$. If not, the wrong value of x_B has been used and a new one should be tried. Again use a tolerance of 0.001.

Nomenclature and Data:

f = fraction of feed which is vapor 0.50
NB = number of ideal plates in stripping section 12
NT = number of ideal plates in rectifying section 16

x_D = mole fraction light component in overhead 0.995
x_F = mole fraction light component in feed 0.60
x_i = mole fraction light component in liquid leaving plate i
x_s = x-coordinate of intersection of feed line and operating lines
y_i = mole fraction light component in vapor leaving plate i
α = relative volatility 1.95

2. Problem Formulation and Technical Analysis: From a material balance the equation for the rectifying operating line can be found to be

$$y_{i+1} = [R_D/(R_D+1)]\,x_i + x_D/(R_D+1). \tag{1}$$

Since the equation for the feed line is

$$y = -(1-f)\,x/f + x_F/f, \tag{2}$$

the value of the x-coordinate (x_s) at the intersection of the rectifying operating line and the feed line is

$$x_s = [x_F/f - x_D/(R_D+1)]/[R_D/(R_D+1) + (1-f)/f]. \tag{3}$$

Thus, if the feed composition (x_F), reflux ratio (R_D), and feed condition (f) are known then the x-coordinate of the feed line - operating line intersection can be determined. y_s is identical with y_{NT+1} where NT represents the number of plates in the rectifying section.

For the stripping section the operating line equation can be represented as a line with slope m.

$$y_i = m(x_{i+1} - x_1) + x_1 \tag{4}$$

where: $m = (y_s - x_1)/(x_s - x_1)$
$= (y_{NT+1} - x_1)/(x_s - x_1)$
i = plate number counting up the column.

The equilibrium relation is stated mathematically as

$$y_i = \alpha x_i/[1 + (\alpha-1)\,x_i] \tag{5}$$

Since x_F, x_D, f, NT and NB are given, the solution to this problem involves finding the value of R_D such that the intersection point (x_s, y_s) is reached after exactly NT stages in the rectifying section. For the stripping section the bottoms composition (x_1) must be found such that the same intersection (x_s, y_s) is reached after NB stages. The problem solution obviously involves trial and error calculations.

3. Method of Solution: To solve this problem it is necessary to use a trial and error process. If a function D is defined as the difference between x_{NT} and x_s in the rectifying section and the difference between x_{NB+1} (plates numbered upward) and x_s in the stripping section, the trial and error calculation amounts to finding the zero root of the function D. Experience has shown that simple linear interpolation and/or extrapolation works excellently for simple trial and error problems. The method of regula falsi (see any numerical analysis text) is such a root finding method. The pertinent relations are more easily derived from the iteration equation for the Newton-Raphson method

$$x_{n+1} = x_n - D(x_n)/D'(x_n) \qquad (6)$$

where the subscripts represent the interation number.

By approximating the derivative D'(x) with the slope of a line passed between the last 2 trial points,

$$D'(x_n) = \frac{D(x_n) - D(x_{n-1})}{x_n - x_{n-1}} ,$$

equation (6) can be rewritten as

$$\Delta X_{n+1} = [-D(x_n)]\, \Delta X_n/[D(x_n) - D(x_{n-1})] \qquad (7)$$

where $\Delta X_{n+1} = x_{n+1} - x_n$

$\Delta X_n = x_n - x_{n-1}$

$D(x_n)$ = function D evaluated for x_n

Equation (7) is useful for a wide variety of problems since it is usually easy to invent a function which is zero at the answer. For example, if the value of x is desired which makes the function $\emptyset(x)$ equal to 9.5 then D could be defined as $\emptyset(x) - 9.5$.

Equation (7) is written in the form of Δx_{n+1} because this eliminates the necessity of writing the basic function twice before the program will begin generating its own new x guesses. This is accomplished by starting the program with $D(x_{n-1})$ equal to zero. This means that the second ΔX (first generated one) is equivalent to minus the first one.

In this problem the variable x_n represents R_D in the rectifying section and x_1 in the stripping section. Note that x_n has no direct relation to the variable x_i which was discussed earlier.

To solve this problem an initial guess is made for R_D and the program proceeds to make changes in R_D depending on how close the computed value of x_{NT} is to x_s. After a match is obtained a similar procedure is conducted for the stripping section except that x_1 is the quantity which is varied.

4. References and Data: This problem is based on an actual industrial problem. "Unit Operations of Chemical Engineering" by McCabe and Smith can be used for further details of equations (1) - (5).

5. Solution:

   a) Results: The results are about as expected.

   b) Discussion of Results: The number of iterations required to find the final answers were 4 for the rectifying section and 6 for the stripping section. This indicates how well linear interpolation works because x_s actually changes with each change in R_D. The method is actually required to hit a "moving target."

III. EDUCATIONAL (PEDOGOLOGICAL) ASPECTS

1. Description of Past Usage: This problem has been used 2 years in a junior-level chemical engineering computer applications course. It would also be useful in a distillation course.

2. Concepts Demonstrated: a) Solution of a trial and error McCabe-Thiele problem with a moderately large number of plates. b) The use of an extremely valuable, yet simple, trial and error procedure.

3. Evaluation of Usage: Students need 1-2 weeks for this unless they have run trial and error programs before.

They seemed pleased to be able to do a more "typical" McCabe-Thiele problem. The information given in this problem is quite typical of many actual situations yet students often aren't assigned this type of problem because the graphical technique is not satisfactory for large numbers of plates. They all realized that this was a problem which would be difficult to solve by any other means.

For advanced students or as a bonus a computer plot could be requested.

4. Nature of Assignment: The information in section II-1 was handed out as a problem statement. Material in II-2 and II-3 was discussed in lecture.

IV. PROGRAM SUMMARY SHEET

V. PROGRAM DESCRIPTION

1. General Description: The program is in two main sections: the rectifying section and the stripping section. Values of NB, NT, f, alpha, x_F and x_D are read in as data. The data is echo printed. An initial guess of 1 is made for R_D and calculations made down the column to the feed plate. At this point a check is made to see if x_{NT} matches the x-coordinate of the intersection of the operating line and feed line. If there is not a match then a new value for R_D is guessed using the linear interpolation process. After a match is obtained the program prints the rectifying section results and then proceeds to the stripping section. To prevent the possibility of bad guesses possibly carrying the stagewise calculations into a negative x range, the calculations are made up the column in the stripping section. This serves to constrain the calculations to acceptable ranges. After the value of x_1 (bottoms composition) has been found which gives a match between x_s and x_{NB+1}, the plate compositions are printed for the stripping section. Contrary to what was done during the calculations, the plate numbers in the stripping section results increase down the column.

2. External and Internal Description: Comment cards provide details for

a) form of data
b) calculation details
c) program nomenclature

No error diagnostics are provided. Program should work for any value of f (feed condition).

VI. PROGRAM LISTING

```
C   BINARY DISTILLATION USING MC CABE-THIELE ASSUMPTIONS.
C***
C
C   MATHEMATICAL TECHNIQUE:
C***
C
C   MAIN PROGRAM
C
C      PURPOSE:
C      READS IN DATA AND CALCULATES THE REFLUX RATIO USING A TRIAL AND
C      ERROR TECHNIQUE.  AFTER THE REFLUX RATIO IS DETERMINED THE BOTTOM
C      COMPOSITION IS DETERMINED BY ANOTHER TRIAL AND ERROR CALCULATION.
C      RESULTS FOR EACH PLATE ARE PRINTED.
C***
C
C      DESCRIPTION OF IMPORTANT VARIABLES:
C
C      ALPHA:  RELATIVE VOLATILITY
C
C      D:  USED IN THE TRIAL AND ERROR CALCULATION TO REPRESENT THE
C      ERROR IN THE FINAL RESULT AFTER EACH TRIAL.  THE OBJECTIVE IS
C      TO DRIVE THIS VARIABLE TO ZERO.  IN THE RECTIFYING SECTION IT
C      REPRESENTS THE DIFFERENCE BETWEEN THE COMPUTED LIQUID COMP.
C      LEAVING THE LOWEST PLATE IN THAT SECTION AND XS.  IN THE
C      STRIPPING SECTION IT IS THE DIFFERENCE BETWEEN THE COMPUTED
C      LIQUID COMPOSITION ENTERING THE TOP PLATE OF THE STRIPPING
C      SECTION AND XS.
C
C      DELB:  REPRESENTS THE SIZE OF THE CHANGE TO BE MADE IN THE
C      BOTTOMS COMPOSITION BEFORE MAKING ANOTHER TRIAL.
C
C      DELR:  REPRESENTS THE SIZE OF THE CHANGE TO BE MADE IN THE
C      REFLUX RATIO BEFORE ANOTHER TRIAL IS MADE.
C
C      DP:  REPRESENTS THE VALUE OF D FOR THE LAST TRIAL PREVIOUS
C      TO THE CURRENT ONE (I.E. THE VALUE FOR THE N-1 ITERATION).
C
C      F:  THE FRACTION OF THE FEED WHICH IS VAPOR.
C
C      NB:  NUMBER OF IDEAL PLATES IN THE STRIPPING (BOTTOM) SECTION.
C
C      NT:  NUMBER OF IDEAL PLATES IN THE RECTIFYING (TOP) SECTION.
C
C      R:  REFLUX RATIO
C
C      SL:  SLOPE OF THE OPERATING LINE IN THE STRIPPING SECTION.
C
C      X:  AN ARRAY TO REPRESENT THE LIQUID COMPOSITION LEAVING THE
C      PLATES.
C
C      XD:  COMPOSITION OF THE OVERHEAD PRODUCT.
C
C      XF:  MOLE FRACTION OF THE LIGHT COMPONENT IN THE FEED.
C
C      XS:  THE X-COORDINATE OF THE INTERSECTION OF THE FEED LINE AND
C      THE OPERATING LINES.
C
C      Y:  AN ARRAY TO REPRESENT THE VAPOR COMPOSITION LEAVING THE
C      PLATES.
```

```
C***
C
C
C
C     DATA INPUT:
C                                  VARIABLES               FORMAT
C         FIRST(ONLY) CARD:     XD,XF,ALPHA,F,NB,NT     4F10.0,2I5
C***
C
C     OUTPUT:
C
C     1.  ECHO PRINT OF INPUT DATA.
C     2.  VALUES OF THE GUESSED VARIABLE (RECTIFYING SECTION: R;
C         STRIPPING SECTION: X(1)) AND THE ERROR AT XS FOR EACH TRIAL.
C     3.  THE LIQUID AND VAPOR COMPOSITIONS FOR EACH PLATE.
C***
C
C     LIMITATIONS:  THE TOLERANCE FOR D HAS BEEN SET TO 0.001.
C
C
C***********************************************************************
C
C
      DIMENSION X(100), Y(100)
      DATA IN,IO/5,6/
    1 FORMAT (4F10.0,2I5)
    2 FORMAT (19H1RECTIFYING SECTION/)
    3 FORMAT (41H0OPERATING LINE INTERSECTS FEED LINE AT =,F7.4)
    4 FORMAT (14H0REFLUX RATIO:,F6.2,4X,6HERROR:,F6.3)
    5 FORMAT (18H0PLATE     X        Y,/(I4,F9.3,F7.3))
    6 FORMAT (/18H1STRIPPING SECTION/)
    7 FORMAT (13H0BOTTOM COMP:F6.3,4X,6HERROR:,F6.3)
    8 FORMAT (10H1DATA ECHO/5H XD =,F7.4,3X,4HXF =,F7.4,/8H ALPHA =,
     1   F6.3,3X,3HF =,F6.3,/5H NB =,I3,4X,4HNT =,I3)
      READ (IN,1) XD, XF, ALPHA, F, NB, NT
      WRITE (IO,8) XD, XF, ALPHA, F, NB, NT
C
C   RECTIFYING SECTION
C
      R = 1
      WRITE (IO,2)
      DP = 0
C   BY SETTING DP = 0 THE FIRST FIRST TIME THE SECOND VALUE OF
C   DELR COMPUTED IN STATEMENT 25 WILL BE MINUS THE FIRST ONE. (SEE
C   OUTPUT).
      DELR = 1
C   NEXT STATEMENT COMPUTES THE NEW VALUE OF THE REFLUX RATIO.
    9 R = R + DELR
      Y(1) = XD
C   THE NEXT STATEMENT CHECKS F.  IF IT IS ZERO THEN XS IS SET
C   EQUAL TO XF AND TRANSFER IS MADE TO STATEMENT 15. THIS AVOIDS
C   DIVISION BY ZERO IN STATEMENT 14.
      IF (F)14,10,14
   10 XS = XF
      GO TO 15
   14 XS = (XF/F-XD/(R+1.))/(R/(R+1.)+(1.-F)/F)
   15 WRITE (IO,3) XS
C   NEXT 4 STATEMENTS PERFORM CALCULATIONS DOWN THE PLATES IN THE
C   RECTIFYING SECTION.
      DO 20 I=1,NT
```

```
C   NEXT STATEMENT IS THE EQUILIBRIUM RELATION
      X(I) = Y(I)/(ALPHA-(ALPHA-1.)*Y(I))
C   FOLLOWING STATEMENT IS THE EQUATION FOR THE RECTIFYING OPER. LINE.
      Y(I+1) = R/(R+1.)*X(I)+XD/(R+1.)
   20 CONTINUE
      D = X(NT)-XS
      IF(ABS(D)-0.001)27,27,25
C   NEXT STATEMENT IS THE COMPUTER REPRESENTATION OF EQN. (7) IN THE
C   WRITE-UP.
   25 DELR = -D*DELR/(D-DP)
      DP = D
      WRITE (IO,4) R, D
      GO TO 9
   27 WRITE (IO,5)(I,X(I),Y(I),I=1,NT)
C
C   STRIPPING SECTION
C
C   FOR EASE IN PROGRAMMING, THE PLATES IN THE STRIPPING SECTION
C   ARE NUMBERED FROM THE BOTTOM UP.  HOWEVER, THEY WILL BE NUMBERED
C   DOWN THE COLUMN IN THE OUTPUT.
      WRITE (IO,6)
      X(1) = 0.005
      DELB = 0.05
      DP = 0
C   NEXT STATEMENT COMPUTES THE NEW VALUE OF THE BOTTOMS COMP.
   30 X(1) = X(1) + DELB
C   THE NEXT 4 STATEMENTS ARE DESIGNED TO PREVENT X(1) FROM BECOMING
C   NEGATIVE.  IF A VALUE OF DELB DRIVES X(1) NEGATIVE THEN DELB IS
C   HALVED AND THIS NEW VALUE IS TRIED.
      IF (X(1))35,35,40
   35 X(1) = X(1) - DELB
      DELB = DELB/2.
      GO TO 30
   40 SL = (Y(NT+1)-X(1))/(XS-X(1))
C   NEXT 4 STATEMENTS PERFORM CALCULATIONS UP THE PLATES IN THE
C   STRIPPING SECTION.
      DO 45 I=1,NB
C   NEXT STATEMENT IS THE EQUILIBRIUM RELATION
      Y(I) = ALPHA*X(I)/(1.+(ALPHA-1.)*X(I))
C   FOLLOWING STATEMENT IS THE EQUATION FOR THE STRIPPING OPERATING LINE
      X(I+1) = (Y(I)-X(1))/SL + X(1)
   45 CONTINUE
      D = X(NB+1)-XS
      IF(ABS(D)-0.001)55,55,50
   50 DELB = -D*DELB/(D-DP)
      DP = D
      WRITE (IO,7) X(1), D
      GO TO 30
C   THE FOLLOWING INVOLVES SOME MANIPULATIONS IN ORDER TO HAVE
C   THE RESULTS IN THE STRIPPING SECTION PRINTED WITH THE PLATE
C   NUMBERS INCREASING DOWN THE COLUMN.  THIS IS NECESSARY BECAUSE
C   THE PLATES WERE NUMBERED UP THE COLUMN DURING THE TRIAL AND ERROR
C   CALCULATIONS.
   55 ISTART = NT + 1
      IEND = NB + NT
      WRITE (IO,5) (I,X(NT+NB-I+1),Y(NT+NB-I+1),I=ISTART,IEND)
      STOP
      END
```

```
                DATA ECHO
                XD = 0.9950    XF = 0.6000
                ALPHA = 1.950    F = 0.500
                NB = 12     NT = 16


RECTIFYING SECTION

OPERATING LINE INTERSECTS FEED LINE AT = 0.5210

REFLUX RATIO:  2.00    ERROR: 0.135

OPERATING LINE INTERSECTS FEED LINE AT = 0.4683

REFLUX RATIO:  1.00    ERROR: 0.475

OPERATING LINE INTERSECTS FEED LINE AT = 0.5318

REFLUX RATIO:  2.40    ERROR: 0.013

OPERATING LINE INTERSECTS FEED LINE AT = 0.5328

REFLUX RATIO:  2.44    ERROR: 0.003

OPERATING LINE INTERSECTS FEED LINE AT = 0.5330

PLATE     X       Y
  1     0.990   0.995
  2     0.984   0.992
  3     0.975   0.987
  4     0.963   0.981
  5     0.948   0.973
  6     0.928   0.962
  7     0.902   0.947
  8     0.870   0.929
  9     0.832   0.906
 10     0.789   0.880
 11     0.743   0.849
 12     0.694   0.816
 13     0.647   0.782
 14     0.604   0.748
 15     0.565   0.717
 16     0.533   0.690
```

```
STRIPPING SECTION

BOTTOM COMP: 0.055    ERROR: 0.035

BOTTOM COMP: 0.005    ERROR:-0.117

BOTTOM COMP: 0.043    ERROR: 0.030

BOTTOM COMP: 0.035    ERROR: 0.025

BOTTOM COMP: 0.017    ERROR:-0.007

BOTTOM COMP: 0.021    ERROR: 0.005

PLATE     X       Y
 17     0.508   0.668
 18     0.471   0.635
 19     0.424   0.590
 20     0.366   0.530
 21     0.301   0.457
 22     0.235   0.375
 23     0.174   0.292
 24     0.123   0.215
 25     0.083   0.150
 26     0.054   0.100
 27     0.033   0.063
 28     0.019   0.037
```

I. PROBLEM IDENTIFICATION

1. Title: Multicomponent Distillation
2. Author: Neil S. Berman
3. Affiliation: Arizona State University

II. TECHNICAL DESCRIPTION

1. Problem statement: The hydrocarbon mixture below is to be separated into a distillate containing 99% of the $i - C_4$ and 2% of the $i - C_5$. The pressure is 120 psia. Find the number of trays, feed tray location, temperature distribution, and compositions of the liquid and vapor on each tray for a reflux ratio of 1.5 times the minimum. The feed is liquid at the bubble point and a total condenser is used.

Component	Mole %
C_3	5
$i - C_4$	15
$n - C_4$	25
$i - C_5$	20
$n - C_5$	35

2. Problem Formulation and Technical Analysis: With $i - C_4$ as the light key and $i - C_5$ as the heavy key the minimum reflux, minimum number of trays and estimates of the end product compositions can be found from approximate methods given in the references. To use the computer program the following information must be available:

   a. Estimates of end product compositions.
   b. Temperatures at the top and bottom of the column.
   c. Liquid and vapor rates in the column.
   d. The number of stages and the feed tray location.

Assume that none of the components heavier than the heavy key appear in the distillate and none lighter than the light key appear in the bottoms. Then Underwood's method is used for the minimum reflux and for the compositions between the keys. The minimum number of trays and the composition at total reflux can be estimated from Fenske's equation. For the specified reflux an estimate can be made by interpolation using the variable R/R+1. The temperature of the distillate and bottoms can be estimated from the dew point and bubble point respectively. Finally the feed can be located at the tray closest in temperature assuming a linear profile. The total number of trays at the specified reflux is determined from the Gilliland chart.

In the given problem the results of such a preliminary analysis are as follows: Minimum reflux ratio, 1.29, minimum number of trays, 8.7, number of trays at a reflux ratio of 2.0 (approximately 1.5 times the minimum), 16.3, and for 17 tray column the composition and amounts of distillate and bottoms are based upon 100 moles of feed.

Component	Distillate = 37.26 X_D	Bottoms = 62.74 X_B
C_3	.1342	.0001
i C_4	.3985	.0023
n C_4	.4563	.1276
i C_5	.0107	.3120
n C_5	.0003	.5580

The top tray temperature is 142 degrees Fahrenheit and the bottom tray 228 degrees Fahrenheit. The feed at 179 degrees would be at the 10th tray from the bottom. To check the column and get more correct compositions and temperatures a plate to plate calculation must be made.

3. Method of solution: A modified Lewis-Matheson method is used for the column iteration. The liquid and vapor flows are assumed constant above and below the feed. To start the temperature profile in the column is assumed to be linear between the top and bottom. The vapor-liquid equilibrium constants are available for each component as a quadratic equation in temperature, $K = E_1 + E_2*T + E_3*T**2$. Let α_i be the relative volatility, K for component i divided by K for the heavy key.

Let V be the vapor flow rate in the top of the column, and VB, the vapor flow rate below the feed. Q will be the liquid flow above the feed and QB, below the feed. D represents the distillate and B the bottoms. $X_{i,m}$ refers to the liquid mole fraction on plate m with a similar definition for $Y_{i,m}$.

The plate to plate calculations start at the top of the column where for a total condenser $Y_{i,N} = X_{i,D}$. Then $X_{i,N}$ can be calculated from the equilibrium constant. However, the sum of the mole fractions in the liquid will not necessarily add up to 1.0, so this condition must be forced by dividing by the sum of the X. For any tray above the feed:

$$\frac{X_{i,N}}{\sum X_{i,n}} = \frac{V*Y_{i,N}/\alpha_i}{\sum V*Y_{i,n}/\alpha_i} \qquad (1)$$

The previously assumed temperature is used to find the equilibrium constants. Next the vapor composition from the previous tray (the top tray has the highest number) can be found from the mass balance:

$$Y_{i,n-1} = \frac{RR}{RR+1} X_{i,n} + \frac{1}{RR+1} X_{i,D} \qquad (2)$$

Where RR is the reflux ratio. At the same time that $X_{i,n}$ and $Y_{i,n-1}$ are calculated for a particular tray, a new temperature can also be determined. First an equilibrium constant for the heavy key is found.

$$K_n = \sum_{i=1}^{NC} Y_{i,n}/\alpha_i \qquad (3)$$

where NC is the total number of components. From the quadratic equation for K a new temperature can be found corresponding to this K. Similar calculations are carried out from the top plate down to and including the feed.

Next the stage calculations are performed from the bottom up. The liquid composition of the bottom tray is the bottoms composition. Then the vapor compositions can be found from the equilibrium constants and normalized so their sum equals 1 as follows:

$$\frac{Y_{i,n}}{\sum Y_{i,n}} = \frac{{}_i{*}X_{i,n}}{\sum \alpha_i{*}X_{i,n}} \qquad (4)$$

From the operating line equation for the trays below the feed the liquid composition of the tray above can be determined.

$$X_{i,n+1} = (VB/QB){*}Y_{i,n} + (B/QB){*}X_{i,1} \qquad (5)$$

A new temperature for the trays below the feed can be determined using the liquid composition similar to the procedure for the trays above the feed.

$$1/K_{\text{heavy key}} = \sum_{i=1}^{NC} \alpha_i{*}X_{i,n} \qquad (6)$$

Calculations are continued until the feed plate is reached from the bottom.

Convergence is slow if the feed compositions calculated from the top down are compared with those from the bottom up. Instead the temperatures will be compared on each tray with the previous iteration and the maximum difference checked with a predetermined standard.

For the next iteration if one is necessary the distillate and bottoms compositions for the components other than the keys will be changed by the following amounts:

$$\Delta(D*X_{i,D}) = \frac{X_{i,bf} - X_{i,df}}{X_{i,df}/(D*X_{i,D}) + X_{i,bf}/(B*X_{i,B})} \tag{7}$$

$$\Delta(B * X_{i,B}) = -D * X_{i,D} \tag{8}$$

If the maximum temperature difference is greater than 0.7 degrees in the example problem, another iteration is made by using the corrections to the distillate and bottoms and the new temperatures. Each iteration is printed and the program converges after 11 iterations. The temperature difference and maximum number of iterations are inputs to the program.

The same program can be used for any guess of operating conditions even if they are not obtained from approximate methods. Then, if convergence cannot be obtained, new choices for RR,N, or feed location can be used. If liquid and vapor flows are not constant heat balances can be added by subscripting the V as V_n and Q as Q_n. In the top of the column the balances

$$Q_{n+1} = V_n - D$$

$$V_n = (D(h_D - h_{n+1}) + (qc) / (H_n - h_{n+1})$$

Where the h and H represent enthalpies of liquid and vapor respectively and qc is the condenser heat load. A similar heat balance can be written for the bottom of the column.

4. References and Data: A similar problem can be found in B. D. Smith. Data for the equilibrium constants are taken from DePriester's curves and fit to a quadratic equation over the range of temperatures for the desired separation.

a. R. E. Treybal, "Mass Transfer Operations," 2nd ed., McGraw-Hill, 1968, pp. 368-390.

b. M. Van Winkle, "Distillation," McGraw-Hill, 1967, pp. 290-321.

c. C. D. Holland, "Multicomponent Distillation," Prentice Hall, 1963.

d. B. D. Smith, "Design of Equilibrium Stage Processes," McGraw-Hill, 1963.

e. DePriester, Chem. Eng. Prog. Symp, Series 7, 49, 1 (1953)

5. Solution:

a. Results: The first and last iterations are shown on the following pages showing that the column will work with the resulting products.

b. Discussion of Results: The Lewis Matheson method presents some computational difficulties, and generally this program will not work without some interaction by the student. The example does converge very nicely using the approximate starting point. There is apparently some difference in the K values used for the approximate calculations and those in the computer program so the compositions are changed considerably. However, if the feed location is shifted the column cannot fit the desired light key and heavy key splits. The student would have to recognize this from the printout and try a new feed tray location or number of trays. The computer program only can change the non-key components and generally will make these fit on the feed tray after 20 iterations. Since a discrete tray sequence is used in a column an exact fit at the feed tray may never be obtained. In spite of these difficulties this method takes up little time on a computer, is easy to write for a specific problem and can be handled in a junior class. An appreciation of some of the difficulties is also desirable for the students.

III. EDUCATIONAL (PEDOGOGICAL ASPECTS)

1. Description of Past Usage: I have used a similar problem in the second semester junior course in Unit Operations for the past three years at Arizona State University. The students all did the preliminary column calculations for homework and then were given the option of the computer stage to stage calculation or taking a test. The problem and solution presented in the past sections is the last one that I assigned representing what I believe is possible for the better students in the class. The students were asked to write the computer program using the time sharing computer and to consider a program only for the problem assigned, not a general multicomponent distillation program.

2. Concepts demonstrated: The students in addition to solving a complex problem are to gain some insight in how to handle a real problem. That is to gather data, examine the problem by approximate procedures to start, and then refine the solution to obtain the final design.

3. Evaluation of usage: In actual practice the best students in class were able to finish the program in a time less than the estimated and generally tried out other conditions beyond those in the original problem. However, the poorest students made little or no progress. They had difficulty using the data and understanding the iterative procedure. Others in the class fell between these extremes. Everyone seemed to gain something from the problem and in general the students developed a real interest. I should add that I have tried to simplify the problem over the years so that the average student can complete it. In my first try several years ago only the best did and he finished at the deadline;

Last year Mr. McKee finished in one week and about 30% of the class handed in almost complete solutions (one or two minor problems generally related to the computer programming). I have never used an absolute grading system where the student must do this problem. They either do this or take a test, therefore, at some point many just stop and take their chances with the test.

4. Nature of Assignment: The students were expected to spend about 20 hours on this in addition to discussions in class. No other homework was assigned during the three week period of this assignment.

IV. PROGRAM SUMMARY SHEET (attached)

V. PROGRAM DESCRIPTION

1. General: The program COMPO tests a preliminary multicomponent distillation column design to see if the desired separation is possible. It is complete within itself with no subroutines. The proposed column must have a total condenser, a reboiler and have the amounts of the heavy key and light key fixed in the distillate and bottoms. The number of trays, reflux ratio, and feed tray location are also fixed. Equilibrium constants, K values, must be supplied as quadratic functions of temperature. The initial trial for top and bottom temperature and distillate and bottoms composition are required inputs.

Vapor and liquid flows above and below the feed are constant. The program checks the maximum temperature change on each tray from the previous iteration and adjusts the distillate and bottoms compositions based on the feed tray differences from the top down and the bottom up.

Further details are supplied in the comment cards.

2. External Description: The comment cards, listed in the next section provide details on data input format and output format. The output consists of an echo print of the input and a complete summary of each iteration up to the number specified or up to convergence within the

temperature difference specified.

3. Internal Description:

a. Program variables - description is given in the comment cards.

b. Program logic - the comment cards follow the program description of Section II.3. To conserve space only one K value evaluation is used but not as a function. Some ordering must be done to include this part of the program in the calculations on both the top and bottom of the column.

c. Diagnostics - none are included. One possible chance for error has been eliminated by setting any small negative value for composition to an arbitrary small positive number. In some cases this number should be even smaller since one or more components may be present in the distillate or bottoms in such a small amount that round-off errors will give equal chance of plus or minus compositions. Minus compositions or zero compositions must be avoided. After enough iterations only positive values should result.

```
      PROGRAM COMPO (INPUT,OUTPUT,TAPE50=INPUT,TAPE66=OUTPUT)
C
C
C     PROGRAM  COMPO                                                    COMP  10
C                                                                       COMP  20
C     MULTICOMPONENT DISTILLATION USING LEWIS MATHESON METHOD           COMP  30
C     THIS PROGRAM WILL TEST A  PRELIMINARY DESIGN TO SEE IF THE        COMP  40
C     DESIRED SEPARATION IS POSSIBLE.  THE AMOUNT OF HEAVY AND          COMP  50
C     LIGHT KEYS IN THE DISTILLATE AND BOTTOMS ARE FIXED.               COMP  60
C     INPUTS TO THE PROGRAM ARE NUMBER OF TRAYS , FEED TRAY LOCATION,   COMP  70
C     DISTILLATE AND BOTTOMS COMPOSITION, REFLUX RATIO, EQUILIBRIUM     COMP  80
C     CONSTANTS AS A QUADRATIC FUNCTION OF TEMPERATURE, AND THE         COMP  90
C     TEMPERATURES AT THE TOP AND THE BOTTOM OF THE COLUMN.             COMP 100
C                                                                       COMP 110
C****                                                                  COMP 120
C     DESCRIPTION OF IMPORTANT VARIABLES                                COMP 130
C****                                                                  COMP 140
C     T(M) = TEMPERATURE AT TRAY M                                      COMP 150
C                                                                       COMP 160
C     XD(I) = MOLE FRACTION OF COMPONENT I IN DISDILLATE                COMP 170
C                                                                       COMP 180
C     XB(I) = MOLE FRACTION OF COMPONENT I IN BOTTOMS                   COMP 190
C                                                                       COMP 200
C     XF(I) = MOLE FRACTION OF COMPONENT I IN FEED                      COMP 210
C                                                                       COMP 220
C     F = MOLES OF FEED                                                 COMP 230
C                                                                       COMP 240
C     D = MOLES OF DISTILLATE                                           COMP 250
C                                                                       COMP 260
C     B = MOLES OF BOTTOMS                                              COMP 270
C                                                                       COMP 280
C     NC = NUMBER OF COMPONENTS                                         COMP 290
C                                                                       COMP 300
C     N = NUMBER OF TRAYS                                               COMP 310
C                                                                       COMP 320
C     NF = FEED TRAY LOCATION FROM THE BOTTOM OF COLUMN                 COMP 330
C                                                                       COMP 340
C     RR = REFLUX RATIO                                                 COMP 350
C                                                                       COMP 360
C     IHK = COMPONENT DESIGNATED HEAVY KEY                              COMP 370
C                                                                       COMP 380
C     ILK = COMPONENT DESIGNATED LIGHT KEY                              COMP 390
C                                                                       COMP 400
C     ISTOP = MAXIMUM NUMBER OF ITERATIONS                              COMP 410
C                                                                       COMP 420
C     X(I,M) = MOLE FRACTION IN LIQUID AT TRAY M                        COMP 430
C                                                                       COMP 440
C     Y(I,M) = MOLE FRACTION IN VAPOR AT TRAY M                         COMP 450
C                                                                       COMP 460
C     EK(I) = K VALUE FOR COMPONENT I AT TEMPERATURE T(M)               COMP 470
C                                                                       COMP 480
C     A(I) = RELATIVE VOLATILITY REFERRED TO HEAVY KEY                  COMP 490
C                                                                       COMP 500
C     E(J,I) = CONSTANTS IN EQUATION FOR EK(I) AS FUNCTION OF T(M)      COMP 510
C                                                                       COMP 520
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C     TDMAX = MAXIMUM TEMPERATURE DIFFERENCE FOR ITERATIONS             COMP 530
C                                                                       COMP 540
C     TTOP = INITIAL TEMPERATURE GUESS FOR DISTILLATE                   COMP 550
C                                                                       COMP 560
C     TBOT = INITIAL TEMPERATUPE GUESS FOR BOTTOMS                      COMP 570
C****                                                                   COMP 580
C     DATA INPUT                                                        COMP 590
C****                                                                   COMP 600
C                       VARIABLES                         FORMAT        COMP 610
C                                                                       COMP 620
C     1. FIRST CARD     NC, N, NF, IHK, ILK               5I5           COMP 630
C                                                                       COMP 640
C     2. SECOND CARD OR                                                 COMP 650
C        SET OF CARDS   F,  XF(I)                         8F10.0        COMP 660
C        IF MORE THAN                                                   COMP 670
C        7 COMPONENTS                                                   COMP 680
C                                                                       COMP 690
C     3. THIRD CARD OR                                                  COMP 700
C        SET            D,  XD(I)                         8F10.0        COMP 710
C                                                                       COMP 720
C     4. FOURTH CARD OR                                                 COMP 730
C        SET            B,  XB(I)                         8F10.0        COMP 740
C                                                                       COMP 750
C     5. NEXT CARD      TTOP, TBOT                        2F10.0        COMP 760
C                                                                       COMP 770
C     6. SIXTH SET      CONSTANTS IN K VALUE                            COMP 780
C                       EQUATION, ONE COMPONENT           3E20.8        COMP 790
C                       PER CARD.                                       COMP 800
C                                                                       COMP 810
C     7. NEXT CARD      REFLUX RATIO                      F10.0         COMP 820
C                                                                       COMP 830
C     8. LAST CARD      ISTOP, TDMAX                      I10, F10.0    COMP 840
C****                                                                   COMP 850
C     OUTPUT                                                            COMP 860
C****                                                                   COMP 870
C     1. COLUMN DESCRIPTION                                             COMP 880
C                                                                       COMP 890
C     2. COMPLETE TEMPERATURE AND COMPOSITION PROFILE                   COMP 900
C        FOR EACH ITERATION UP TO ISTOP                                 COMP 910
C****                                                                   COMP 920
C     LIMITATIONS                                                       COMP 930
C****                                                                   COMP 940
C     N MUST BE 30 OR LESS. NUMBER OF COMPONENTS, 10 OR LESS. THE       COMP 950
C     EQUATION FOR K VALUES MUST BE A QUADRATIC WITH THE COEFFICIENT    COMP 960
C     OF THE T**2 TERM NOT EQUAL TO ZERO. ALTHOUGH THIS PROGRAM IS      COMP 970
C     FOR ANY MULTICOMPONENT MIXTURE, THE PROGRAM IS LIMITED TO THE     COMP 980
C     CASE WHERE THE AMOUNTS OF HEAVY AND LIGHT KEYS ARE FIXED IN THE   COMP 990
C     DISTILLATE AND BOTTOMS , TOTAL CONDENSER AND REBOILER ARE USED    COMP1000
C     AND VAPOR AND LIQUID FLOWS ARE CONSTANT ABOVE AND BELOW THE       COMP1010
C     FEED.                                                             COMP1020
C                                                                       COMP1030
C                                                                       COMP1040
C                                                                       COMP1050
      DIMENSION T(30),XD(10),XB(10),XF(10),DELXD(10),DELXB(10),EK(10),  COMP1060
     1E(3,10),Y(10,30),X(10,30),A(10),DF(10),BF(10),DELT(30),XDMOL(10),XCOMP1070
     2PMOL(10)                                                          COMP1080
      DATA IN,IO/50,66/                                                 COMP1090
C     READ NC, N, NF, IHK, ILK                                          COMP1100
    1 READ(IN,101) NC,N,NF,IHK,ILK                                      COMP1110
C     READ FEED AMOUNT AND COMPOSITION                                  COMP1120
    2 READ(IN,102)F,(XF(I),I=1,NC)                                      COMP1130
C     READ DISTILLATE AMOUNT AND COMPOSITION                            COMP1140
    3 READ(IN,102) D,(XD(I),I=1,NC)                                     COMP1150
C     READ BOTTOMS AMOUNT AND COMPOSITION                               COMP1160
    4 READ(IN,102) B,(XB(I),I=1,NC)                                     COMP1170
C     READ TEMPERATURE GUESS FOR TOP AND BOTTOM OF COLUMN               COMP1180
    5 READ(IN,103) TTOP,TBOT                                            COMP1190
C     READ CONSTANTS IN K VALUE QUADRATIC EQUATION                      COMP1200
      DO 6 I=1,NC                                                       COMP1210
    6 READ(IN,104) (E(J,I),J=1,3)                                       COMP1220
C     READ REFLUX RATIO                                                 COMP1230
    7 READ (IN,105) RR                                                  COMP1240
C     READ ISTOP AND TDMAX                                              COMP1250
    8 READ(IN,106)ISTOP, TDMAX                                          COMP1260
C     ECHO PRINT OF INPUT                                               COMP1270
      WRITE(IO,299)                                                     COMP1280
      WRITE(IO,230)                                                     COMP1290
      WRITE(IO,101)NC,N,NF,IHK,ILK                                      COMP1300
      WRITE(IO,216) F,(XF(I),I=1,NC)                                    COMP1310
      WRITE(IO,216) D, (XD(I),I=1,NC)                                   COMP1320
      WRITE(IO,216) B, (XB(I),I=1,NC)                                   COMP1330
      WRITE(IO,220) TTOP, TBOT                                          COMP1340
      WRITE(IO,221) ILK, IHK                                            COMP1350
      DO 9 I=1,NC                                                       COMP1360
    9 WRITE(IO,104) (E(J,I),J=1,3)                                      COMP1370
      WRITE(IO,242)TDMAX, ISTOP                                         COMP1380
C     PRINT COLUMN DESCRIPTION                                          COMP1390
      WRITE (IO,201) NC                                                 COMP1400
      WRITE (IO,202) N,NF                                               COMP1410
      WRITE (IO,203) F,RR                                               COMP1420
      WRITE (IO,204)                                                    COMP1430
      WRITE (IO,205)                                                    COMP1440
C     SET A LINEAR TEMPERATURE PROFILE                                  COMP1450
      TD = N-1                                                          COMP1460
      TGRAD = (TBOT-TTOP)/TD                                            COMP1470
      DO 10 J=1,N                                                       COMP1480
      TN = J-1                                                          COMP1490
   10 T(J) = TBOT - (TN*TGRAD)                                          COMP1500
      IT = 0                                                            COMP1510
C     INITIALIZE DELTAS FOR DISTILLATE AND BOTTOMS                      COMP1520
      DO 12 I=1,NC                                                      COMP1530
      DELXD(I) = 0.0                                                    COMP1540
   12 DELXB(I) = 0.0                                                    COMP1550
C     SET VAPOR AT TOP EQUAL TO DISTILLATE COMPOSITION                  COMP1560
   20 DO 21 I = 1,NC                                                    COMP1570
   21 Y(I,N) = XD(I)                                                    COMP1580
C     SET VALUES OF LIQUID, Q, AND VAPOR, V, FLOWS                      COMP1590
      Q = RR*D                                                          COMP1600
      V = Q+D                                                           COMP1610
      VB = V                                                            COMP1620
```

```
          QB = Q + F                                                              COMP1530
C         PLATE TO PLATE FROM TOP TO FEED SET INITIAL COUNTERS                    COMP1640
          LM = 1                                                                  COMP1650
          M = N                                                                   COMP1660
C         CALCULATION OF RELATIVE VOLATILITY FOR ANY PLATE                        COMP1670
       22 DO 24 I=1,NC                                                            COMP1680
          EK(I)=E(1,I)+E(2,I)*T(M)+E(3,I)*T(M)*T(M)                               COMP1690
       24 CONTINUE                                                                COMP1700
          DO 25 I=1,NC                                                            COMP1710
       25 A(I) = EK(I)/EK(IHK)                                                    COMP1720
          IF(LM.EQ.2)GO TO 50                                                     COMP1730
          IF(M.LT.NF)GO TO 50                                                     COMP1740
C         CALCULATION OF COMPOSITIONS IN PLATES ABOVE FEED                        COMP1750
          SUM = 0.0                                                               COMP1760
          DO 30 I=1,NC                                                            COMP1770
       30 SUM = SUM + Y(I,M)/A(I)                                                 COMP1780
          DO 31 I = 1,NC                                                          COMP1790
       31 X(I,M) = Y(I,M)/(A(I)*SUM)                                              COMP1800
          DO 32 I = 1,NC                                                          COMP1810
       32 Y(I,M-1) = (RR/(RR+1.))*X(I,M)+(1./(RR+1.))*Y(I,N)                      COMP1820
C         NEW TEMPERATURE ON PLATES ABOVE FEED                                    COMP1830
          C = E(1,IHK) - SUM                                                      COMP1840
          TNEW = (-E(2,IHK)+SQRT(E(2,IHK)**2-4.*E(3,IHK)*C))/(2.*E(3,IHK))        COMP1850
          DELT(M) = ABS(TNEW-T(M))                                                COMP1860
          T(M) = TNEW                                                             COMP1870
          M = M-1                                                                 COMP1880
          IF(M.LT.NF)GO TO 40                                                     COMP1890
       39 GO TO 22                                                                COMP1900
C         PLATE TO PLATE FROM BOTTOM UP TO FEED SET COUNTER                       COMP1910
       40 M = 1                                                                   COMP1920
C         SET LIQUID AT PLATE 1 EQUAL TO BOTTOMS COMPOSITION                      COMP1930
C         AND PRESERVE FEED COMPOSITIONS AS CALCULATED FROM TOP DOWN              COMP1940
          DO 41 I=1,NC                                                            COMP1950
          X(I,1) = XB(I)                                                          COMP1960
       41 DF(I) = X(I,NF)                                                         COMP1970
          GO TO 22                                                                COMP1980
C         CALCULATION OF COMPOSITION IN PLATES BELOW FEED                         COMP1990
       50 SUMQ = 0.0                                                              COMP2000
          DO 52 I = 1,NC                                                          COMP2010
       52 SUMQ = SUMQ + A(I)*X(I,M)                                               COMP2020
          DO 54 I = 1,NC                                                          COMP2030
       54 Y(I,M) = A(I)*X(I,M)/SUMQ                                               COMP2040
          IF(M.EQ.NF)GO TO 57                                                     COMP2050
          DO 56 I=1,NC                                                            COMP2060
       56 X(I,M+1) = (VB/QB)*Y(I,M) + (B/QB)*X(I,1)                               COMP2070
C         NEW TEMPERATURE ON PLATES BELOW FEED                                    COMP2080
       57 C = E(1,IHK) - (1.0/SUMQ)                                               COMP2090
          TNEW = (-E(2,IHK)+SQRT(E(2,IHK)**2-4.*E(3,IHK)*C))/(2.*E(3,IHK))        COMP2100
          DELT(M) = ABS(TNEW-T(M))                                                COMP2110
          T(M) = TNEW                                                             COMP2120
          M = M+1                                                                 COMP2130
          IF(M-NF)22,60,61                                                        COMP2140
C         SET COUNTER LM WHEN FEED PLATE IS REACHED FROM BOTTOM UP                COMP2150
       60 LM = 2                                                                  COMP2160
          GO TO 22                                                                COMP2170
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C     STORE FEED COMPOSITIONS FROM BOTTOM UP CALCULATIONS               COMP2180
   61 DO 62 I = 1,NC                                                    COMP2190
   62 DF(I) = X(I,NF)                                                   COMP2200
C     CORRECT DISTILLATE AND BOTTOMS COMPOSITIONS                       COMP2210
      DELXD(ILK) = 0.0                                                  COMP2220
      DELXD(IHK) = 0.0                                                  COMP2230
      SUMD = 0.0                                                        COMP2240
      SUMB = 0.0                                                        COMP2250
      DO 64 I=1,NC                                                      COMP2260
      IF(I.EQ.ILK.OR.I.EQ.IHK) GO TO 63                                 COMP2270
      DELXD(I) = (BF(I) - DF(I))/(DF(I)/(XD(I)*D)+BF(I)/(XB(I)*B))      COMP2280
   63 DELXB(I) = -DELXD(I)                                              COMP2290
      XDMOL(I) = XD(I)*D + DELXD(I)                                     COMP2300
      SUMD = SUMD + XDMOL(I)                                            COMP2310
      XBMOL(I) = XB(I)*B + DELXB(I)                                     COMP2320
      SUMB = SUMB + XBMOL(I)                                            COMP2330
   64 CONTINUE                                                          COMP2340
      D = SUMD                                                          COMP2350
      B = SUMB                                                          COMP2360
      DO 66 I = 1,NC                                                    COMP2370
      XD(I) = XDMOL(I)/D                                                COMP2380
      XB(I) = XBMOL(I)/B                                                COMP2390
      IF(XD(I).LT.0.0)XD(I) = 0.00001                                   COMP2400
      IF(XB(I).LT.0.0)XB(I) = 0.00001                                   COMP2410
   66 CONTINUE                                                          COMP2420
C     CHANGE ITERATION COUNTER                                          COMP2430
      IT = IT + 1                                                       COMP2440
C     PRINT COMPLETE PLATE TO PLATE COMPOSITIONS                        COMP2450
      WRITE(IO,299)                                                     COMP2460
      WRITE(IO,210)IT                                                   COMP2470
      WRITE(IO,211)                                                     COMP2480
      DO 70 J=1,N                                                       COMP2490
   70 WRITE(IO,212)J,T(J), (X(I,J),I=1,NC)                              COMP2500
      WRITE(IO,213)                                                     COMP2510
      DO 72 J=1,N                                                       COMP2520
   72 WRITE(IO,212)J,T(J),(Y(I,J),I=1,NC)                               COMP2530
C     CHECK MAXIMUM TEMPERATURE CHANGE BETWEEN ITERATIONS               COMP2540
      IC = 1                                                            COMP2550
      II = 1                                                            COMP2560
      JJ = 1                                                            COMP2570
   80 DMAX = DELT(II) - DELT(II+JJ)                                     COMP2580
      IF(DMAX.LT.0.)II = II + JJ                                        COMP2590
      IF(DMAX.LT.0.)JJ=1                                                COMP2600
      IF(DMAX.GE.0.)JJ=JJ+1                                             COMP2610
      IC = IC + 1                                                       COMP2620
      IF(IC.EQ.N)GO TO 81                                               COMP2630
      GO TO 80                                                          COMP2640
   81 DMAX = DELT(II)                                                   COMP2650
C     PRINT MAXIMUM TEMPERATURE CHANGE AND NEW DISTILLATE AND BOTTOMS   COMP2660
      WRITE(IO,214)DMAX                                                 COMP2670
      WRITE(IO,215)                                                     COMP2680
      WRITE(IO,216)D,(XD(I),I=1,NC)                                     COMP2690
      WRITE(IO,216)B,(XB(I),I=1,NC)                                     COMP2700
      WRITE(IO,217)                                                     COMP2710
      WRITE(IO,218) (DF(I),I=1,NC)                                      COMP2720
      WRITE(IO,219) (BF(I),I=1,NC)                                      COMP2730
C     STOP IF ISTOP ITERATIONS OR MAX TEMPERATURE CHANGE LESS THAN TDMAXCOMP2740
      IF(IT.EQ.ISTOP)GO TO 98                                           COMP2750
      IF(DMAX.GT.TDMAX)GO TO 20                                         COMP2760
      GO TO 99                                                          COMP2770
   98 WRITE(IO,241)TDMAX,ISTOP                                          COMP2780
   99 GO TO 1                                                           COMP2790
C                                                                       COMP2800
  101 FORMAT (5I5)                                                      COMP2810
  102 FORMAT (8F10.0)                                                   COMP2820
  103 FORMAT (2F10.0)                                                   COMP2830
  104 FORMAT (3E20.8)                                                   COMP2840
  105 FORMAT (F10.0)                                                    COMP2850
  106 FORMAT(I10,F10.0)                                                 COMP2860
  201 FORMAT (//,23H DISTILLATION COLUMN   ,I2,11H COMPONENTS)          COMP2870
  202 FORMAT (/,2X,I2,20H TRAYS WITH FEED ON ,I2,12H FROM BOTTOM)       COMP2880
  203 FORMAT (/,2X,6HBASIS ,F10.4,12H MOLES FEED ,14H REFLUX RATIO ,F10.COMP2890
     14)                                                                COMP2900
  204 FORMAT (/,2X,39H THE FEED IS LIQUID AT THE BUBBLE POINT)          COMP2910
  205 FORMAT (/,2X,23H WITH A TOTAL CONDENSER)                          COMP2920
  210 FORMAT (//,2X,15H FOR ITERATION ,I2)                              COMP2930
  211 FORMAT (2X,36H TEMPEPATURE AND LIQUID COMPOSITIONS,/)             COMP2940
  212 FORMAT (1X,I2,F7.2,7F10.4)                                        COMP2950
  213 FORMAT (/,2X,35H TEMPERATURE AND VAPOR COMPOSITIONS,/)            COMP2960
  214 FORMAT (//,2X,28H MAXIMUM TEMPERATURE CHANGE ,F10.4)              COMP2970
  215 FORMAT (2X,27H NEW DISTILLATE AND BOTTOMS,/)                      COMP2980
  216 FORMAT (8F10.4)                                                   COMP2990
  217 FORMAT (/,2X,29HFEED TRAY LIQUID COMPOSITIONS)                    COMP3000
  218 FORMAT (/,10H  TOP     ,7F10.4)                                   COMP3010
  219 FORMAT (/,10H  BOTTOM  ,7F10.4)                                   COMP3020
  220 FORMAT (2F10.4)                                                   COMP3030
  221 FORMAT (2X,11HLIGHT KEY  ,I2,14H   HEAVY KEY  ,I2)                COMP3040
  230 FORMAT(2X,17H ECHO PRINT INPUT)                                   COMP3050
  241 FORMAT(/,23H NO CONVERGENCE WITHIN ,F10.6,11H DEGREES IN,I5,11H ITCOMP3060
     1ERATIONS)                                                         COMP3070
  242 FORMAT(/,12H CONVERGENCE,F10.6,12H DEGREES AND,I5,11H ITERATIONS) COMP3080
  299 FORMAT(1H1)                                                       COMP3090
      END                                                               COMP3100
```

```
 ECHO PRINT  INPUT
  5   17   10    4    2
100.0000      .0500     .1500      .2500      .2000      .3500
 37.2500      .1342     .3985      .4563      .0107      .0003
 62.7400      .0001     .0023      .1276      .3120      .5580
142.0000  228.0000
LIGHT KEY    2   HEAVY KEY    4
      .14839288E+00         .11098214E-01         .30803572E-04
      .38511872E-01         .34553575E-02         .29613094E-04
      .40833335E+00        -.27738097E-02         .40476191E-04
      .24464281E+00        -.26309158E-02         .25595236E-04
      .16482146E+00        -.20089289E-02         .21875001E-04

CONVERGENCE    .700000 DEGREES AND    30 ITERATIONS


DISTILLATION COLUMN    5 COMPONENTS

 17 TRAYS WITH FEED ON 10 FROM BOTTOM

 BASIS   100.0000 MOLES FEED  REFLUX RATIO      2.0000

  THE FEED IS LIQUID AT THE BUBBLE POINT

  WITH A TOTAL CONDENSER
```

```
FOR ITERATION  1
TEMPERATURE AND LIQUID COMPOSITIONS

 1 225.77      .0001      .0023      .1276      .3120      .5580
 2 218.25      .0003      .0042      .1964      .3031      .4960
 3 211.43      .0008      .0068      .2626      .2849      .4449
 4 205.69      .0020      .0098      .3187      .2641      .4055
 5 200.89      .0047      .0132      .3602      .2452      .3767
 6 196.48      .0108      .0169      .3863      .2298      .3563
 7 191.41      .0239      .0208      .3968      .2175      .3411
 8 184.17      .0513      .0243      .3898      .2067      .3279
 9 173.20      .1038      .0266      .3606      .1954      .3136
10 157.84      .1902      .0262      .3056      .1818      .2962
11 170.86      .0203      .1789      .4288      .3431      .0289
12 165.45      .0214      .1986      .4864      .2737      .0198
13 160.27      .0227      .2210      .5396      .2041      .0127
14 155.60      .0241      .2463      .5804      .1417      .0076
15 151.38      .0268      .2760      .6016      .0914      .0042
16 147.06      .0341      .3130      .5968      .0540      .0021
17 141.07      .0579      .3578      .5555      .0279      .0009

TEMPERATURE AND VAPOR COMPOSITIONS

 1 225.77      .0004      .0053      .2350      .2981      .4612
 2 218.25      .0012      .0093      .3385      .2696      .3815
 3 211.43      .0031      .0140      .4259      .2372      .3199
 4 205.69      .0073      .0193      .4908      .2077      .2750
 5 200.89      .0168      .0251      .5314      .1836      .2430
 6 196.48      .0373      .0311      .5478      .1645      .2193
 7 191.41      .0800      .0367      .5370      .1477      .1987
 8 184.17      .1620      .0403      .4914      .1299      .1765
 9 173.20      .2969      .0395      .4056      .1088      .1493
10 157.84      .4724      .0333      .2917      .0849      .1177
11 170.86      .0590      .2653      .4764      .1861      .0133
12 165.45      .0598      .2802      .5118      .1396      .0086
13 160.27      .0608      .2970      .5390      .0980      .0052
14 155.60      .0626      .3169      .5532      .0645      .0029
15 151.38      .0675      .3415      .5500      .0395      .0015
16 147.06      .0833      .3713      .5224      .0222      .0007
17 141.07      .1342      .3985      .4563      .0107      .0003


MAXIMUM TEMPERATURE CHANGE    18.2114
NEW DISTILLATE AND BOTTOMS

36.1924      .1383      .4103      .4381      .0110      .0023
63.8076      .0000      .0023      .1434      .3068      .5475

FEED TRAY LIQUID COMPOSITIONS

TOP            .0193      .1624      .3746      .4041      .0395

BOTTOM         .1902      .0262      .3056      .1818      .2962
```

```
  FOR ITERATION  2
  TEMPERATURE AND LIQUID COMPOSITIONS

  1 224.14      .0000       .0023       .1434       .3068       .5475
  2 216.27      .0000       .0041       .2172       .2953       .4833
  3 209.49      .0001       .0064       .2855       .2759       .4321
  4 204.18      .0002       .0091       .3408       .2555       .3944
  5 200.29      .0004       .0122       .3809       .2382       .3683
  6 197.46      .0010       .0156       .4070       .2252       .3512
  7 195.19      .0023       .0192       .4224       .2161       .3400
  8 192.86      .0051       .0233       .4296       .2097       .3323
  9 189.60      .0114       .0279       .4302       .2046       .3259
 10 186.61      .0257       .0329       .4232       .1994       .3188
 11 177.62      .0188       .1612       .3514       .2867       .1819
 12 170.76      .0202       .1843       .4152       .2460       .1343
 13 163.91      .0219       .2121       .4805       .1944       .0911
 14 157.73      .0239       .2437       .5353       .1406       .0565
 15 152.42      .0271       .2796       .5685       .0929       .0320
 16 147.38      .0350       .3214       .5716       .0555       .0165
 17 140.73      .0597       .3693       .5348       .0289       .0073

  TEMPERATURE AND VAPOR COMPOSITIONS

  1 224.14      .0000       .0052       .2636       .2886       .4455
  2 216.27      .0001       .0089       .3689       .2578       .3643
  3 209.49      .0003       .0132       .4568       .2254       .3044
  4 204.18      .0007       .0180       .5204       .1979       .2630
  5 200.29      .0016       .0234       .5619       .1773       .2358
  6 197.46      .0036       .0292       .5863       .1629       .2180
  7 195.19      .0091       .0357       .5978       .1526       .2058
  8 192.86      .0180       .0430       .5987       .1445       .1957
  9 189.60      .0407       .0510       .5877       .1362       .1844
 10 186.61      .0858       .0570       .5531       .1286       .1756
 11 177.62      .0596       .2596       .4228       .1677       .0903
 12 170.76      .0607       .2781       .4664       .1333       .0615
 13 163.91      .0620       .2992       .5029       .0974       .0385
 14 157.73      .0641       .3231       .5250       .0656       .0221
 15 152.42      .0694       .3510       .5271       .0407       .0117
 16 147.38      .0859       .3830       .5025       .0229       .0057
 17 140.73      .1383       .4103       .4381       .0110       .0023


  MAXIMUM TEMPERATURE CHANGE     16.3971
  NEW DISTILLATE AND BOTTOMS

  38.2242       .1310       .3884       .4672       .0104       .0030
  61.7758       .0000       .0023       .1157       .3169       .5651

 FEED TRAY LIQUID COMPOSITIONS

 TOP            .0166       .1397       .2936       .3152       .2349

 BOTTOM         .0257       .0329       .4232       .1994       .3188
```

```
FOR ITERATION  3
TEMPERATURE AND LIQUID COMPOSITIONS

 1 226.97     .0000     .0023     .1157     .3169     .5651
 2 219.60     .0000     .0044     .1811     .3099     .5046
 3 212.64     .0001     .0072     .2473     .2924     .4530
 4 206.71     .0002     .0108     .3064     .2711     .4116
 5 202.09     .0004     .0151     .3529     .2509     .3807
 6 198.64     .0039     .0200     .3854     .2346     .3591
 7 196.02     .0021     .0255     .4053     .2225     .3446
 8 193.72     .0048     .0316     .4149     .2140     .3347
 9 191.04     .0109     .0382     .4157     .2076     .3276
10 186.98     .0242     .0451     .4074     .2022     .3211
11 178.81     .0180     .1521     .3669     .2507     .2123
12 172.01     .0193     .1725     .4314     .2176     .1592
13 165.10     .0207     .1973     .4981     .1741     .1098
14 158.83     .0224     .2259     .5550     .1275     .0692
15 153.44     .0253     .2589     .5910     .0851     .0398
16 148.38     .0326     .2983     .5971     .0514     .0207
17 141.79     .0557     .3451     .5628     .0270     .0093

TEMPERATURE AND VAPOR COMPOSITIONS

 1 226.97     .0000     .0055     .2163     .3061     .4720
 2 219.60     .0001     .0099     .3182     .2793     .3926
 3 212.64     .0002     .0154     .4091     .2464     .3289
 4 206.71     .0006     .0220     .4807     .2154     .2814
 5 202.09     .0014     .0295     .5307     .1902     .2482
 6 198.64     .0032     .0379     .5613     .1717     .2258
 7 195.02     .0074     .0473     .5761     .1585     .2107
 8 193.72     .0168     .0575     .5773     .1488     .1996
 9 191.04     .0372     .0682     .5645     .1404     .1897
10 186.98     .0804     .0780     .5330     .1309     .1777
11 178.81     .0565     .2445     .4433     .1486     .1071
12 172.01     .0574     .2610     .4878     .1196     .0742
13 165.10     .0586     .2801     .5257     .0885     .0471
14 158.83     .0605     .3021     .5497     .0602     .0275
15 153.44     .0654     .3284     .5538     .0378     .0148
16 148.38     .0808     .3596     .5309     .0215     .0072
17 141.79     .1310     .3884     .4672     .0104     .0030


MAXIMUM TEMPERATURE CHANGE      3.3321
NEW DISTILLATE AND BOTTOMS

39.5101       .1267     .3758     .4839     .0101     .0035
60.4899       .0000     .0024     .0974     .3236     .5767

FEED TRAY LIQUID COMPOSITIONS

TOP           .0172     .1371     .3134     .2693     .2629

BOTTOM        .0242     .0451     .4074     .2022     .3211
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FOR ITERATION 11
TEMPERATURE AND LIQUID COMPOSITIONS

 1 233.95     .0000     .0025     .0527     .3399     .6049
 2 229.27     .0000     .0050     .0880     .3469     .5600
 3 223.81     .0000     .0091     .1316     .3416     .5177
 4 217.82     .0001     .0151     .1808     .3265     .4775
 5 211.72     .0002     .0237     .2312     .3050     .4400
 6 205.97     .0004     .0350     .2768     .2812     .4065
 7 200.83     .0011     .0491     .3127     .2586     .3785
 8 196.31     .0028     .0660     .3359     .2392     .3562
 9 192.04     .0067     .0852     .3456     .2236     .3389
10 187.18     .0157     .1061     .3420     .2111     .3251
11 180.56     .0161     .1334     .3880     .1977     .2647
12 173.79     .0172     .1508     .4552     .1745     .2024
13 166.91     .0184     .1719     .5253     .1420     .1425
14 160.66     .0199     .1963     .5865     .1057     .0916
15 155.33     .0224     .2248     .6272     .0718     .0537
16 150.43     .0287     .2599     .6387     .0442     .0285
17 144.14     .0494     .3039     .6099     .0237     .0131

TEMPERATURE AND VAPOR COMPOSITIONS

 1 233.95     .0000     .0062     .1040     .3501     .5397
 2 229.27     .0000     .0120     .1673     .3424     .4783
 3 223.81     .0001     .0208     .2389     .3204     .4198
 4 217.82     .0002     .0332     .3120     .2892     .3653
 5 211.72     .0006     .0497     .3783     .2547     .3168
 6 205.97     .0016     .0702     .4303     .2218     .2760
 7 200.83     .0040     .0947     .4641     .1936     .2436
 8 196.31     .0097     .1227     .4783     .1709     .2185
 9 192.04     .0228     .1529     .4730     .1528     .1985
10 187.18     .0520     .1830     .4475     .1370     .1805
11 180.56     .0508     .2172     .4762     .1194     .1364
12 173.79     .0516     .2313     .5229     .0978     .0964
13 166.91     .0526     .2475     .5637     .0736     .0625
14 160.66     .0543     .2666     .5909     .0510     .0373
15 155.33     .0585     .2900     .5985     .0326     .0204
16 150.43     .0723     .3193     .5793     .0189     .0102
17 144.14     .1180     .3501     .5181     .0094     .0043

MAXIMUM TEMPERATURE CHANGE          .6649
NEW DISTILLATE AND BOTTOMS

42.4888       .1178     .3495     .5190     .0094     .0044
57.5112       .0000     .0025     .0514     .3404     .6057

FEED TRAY LIQUID COMPOSITIONS

TOP           .0153     .1202     .3324     .2095     .3227

BOTTOM        .0157     .1061     .3420     .2111     .3251
```

I. PROBLEM IDENTIFICATION

1. Title: Multicomponent Distillation Column Design
2. Author: Orville C. Sandall
3. Affiliation: University of California, Santa Barbara

II. TECHNICAL DESCRIPTION

1. Problem Statement: You are asked to design a distillation column to fractionate a saturated liquid feed having the composition given in the table below. The distillate product is to contain 95% of the n-butane and a bottoms product containing 95% of the isopentane is desired. For these initial calculations a column pressure of 125 psia and a reflux rate of 1.25 times the minimum are chosen as the operating conditions. The feed will be a saturated liquid.

a. For these preliminary calculations a constant relative volatility will be assumed and you are, therefore, asked to estimate the relative volatilities to use in the calculations.

b. Estimate the minimum number of stages required.

c. Estimate the minimum reflux rate.

d. Use the Gilliland correlation to estimate the number of theoretical stages required for the separation.

e. Estimate the approximate location of the feed plate.

f. Use the number of stages calculated in part (d) and the location of the feed tray as determined in part (e) to carry out plate-to-plate calculations using the Lewis-

Matheson method in order to check the specified recovery of the key components.

Component	Mole Fraction in Feed
isobutane	0.05
n-butane	0.20
isopentane	0.35
n-pentane	0.40

2. Problem Formulation and Technical Analysis:

Basis: 100 moles of feed.

a. The average relative volatilities used in the calculations were taken to be the arithmetic average of the relative volatilities corresponding to the temperature at the top of the column and the temperature at the bottom of the column. The temperature at the top of the column is estimated from a dew point calculation based on an assumed distillate product composition; the temperature at the bottom of the column is estimated from a bubble point calculation based on an assumed bottoms product composition. Raoult's law for ideal liquid behavior and Dalton's law for ideal gas behavior are assumed to hold for these vapor-liquid equilibrium calculations. The estimated distillate composition is obtained by assuming that the distillate contains the specified amounts of the key components, all of the component lighter than the light key and none of the component heavier than the heavy key.

The bottoms product composition is estimated in a similar fashion. The results of these calculations are shown in Table I.

TABLE I

AVERAGE RELATIVE VOLATILITY CALCULATIONS

Component	x_D	α_{Top} ($T = 346°K$)	x_B	α_{Bottom} ($T = 386°K$)	α_{mean}
i-butane	0.194	2.92	0.000	2.58	2.75
n-butane	0.736	2.24	0.0135	1.98	2.11
i-pentane	0.070	1.00	0.448	1.00	1.00
n-pentane	0.000	0.787	0.539	0.811	0.80

b. The minimum number of stages, corresponding to total reflux, is calculated from the Fenske equation to be 7.84.

c. The Underwood equations are used to estimate the minimum reflux rate as being 2.33 for the specified separation.

d. The Gilliland correlation (1) is used together with the results of parts (b) and (c) in order to obtain an estimate for the total number of stages required for the specified reflux ratio. The total number of stages required is estimated to be 16.

e. The estimated optimum location of the feed plate is calculated from the Kirkbride equation (2) to be the seventh stage from the top.

f. Before the plate-to-plate calculations can proceed, it is necessary that estimates be made for the composition of components lighter than the light key in the bottoms product and for components heavier than the heavy key in the distillate product. The Fenske equation is applied to each of these components to give their product compositions. The estimated compositions of the bottoms and distillate products are shown in Table II.

TABLE II

ESTIMATED PRODUCT COMPOSITIONS

Component	Mole Fraction in Distillate	Mole Fraction in Bottoms
i-butane	0.190	0.0005
n-butane	0.729	0.0135
i-pentane	0.069	0.449
n-pentane	0.012	0.537

3. Method of Solution: With the assumed product compositions, the plate-to-plate calculations proceed in the following manner:

a. Starting from the assumed distillate composition, the liquid composition on the first stage is calculated from a dew point calculation using the assumed constant relative volatilities.

b. The composition of the vapor leaving the second stage is calculated from material balances.

c. Steps a. and b. are repeated until the liquid on the feed tray is reached.

d. Starting from the assumed bottoms composition, the vapor composition leaving the reboiler is calculated from a bubble point calculation.

e. The composition of the liquid leaving the bottom plate is calculated from material balances.

f. Steps d. and e. are repeated until the liquid on the feed tray is reached.

g. If the compositions of the liquid on the feed plate as calculated from the top down and the bottom up do not match, new product distributions are estimated using the method of Bonner (3) and the calculations are repeated.

According to the method of Bonner the moles of each component in the distillate should be adjusted an amount, Δd, where Δd is given by the formula

$$\Delta d = \frac{x_B - x_T}{x_B/b + x_T/d}$$

where: x_B is the composition of component i in the liquid on the feed plate as calculated from the bottom;

x_T is the composition of component i in the liquid on the feed plate as calculated from the top;

b is the moles of component i in the bottoms product;
d is the moles of component i in the distillate product.

A feed plate match criteria of 0.0001 mole fraction for each component was taken for the calculations.

4. References:

1. C. S. Robinson and E. R. Gilliland, "Elements of Fractional Distillation", 4th ed., McGraw-Hill Book Co., Inc., New York, pp. 347-350, (1950).

2. C. G. Kirkbride, Petroleum Refiner, 23, 321 (1944).

3. J. S. Bonner, Proc. Am. Petrol. Inst., 36, section III, 238 (1956).

5. Solution: The results are shown as computer output entitled "Calculated Results". As shown, a total of 13 iterations were required for convergence. It was found for all cases tested that approximately 10 iterations are required. It may be seen from the results printed out that 16 stages do not meet the specified recovery criteria for the key components. It was found 19 stages are required with the feed introduced on the 10th stage from the top.

III. EDUCATIONAL ASPECTS

1. Description of Past Usage: Students are given two weeks for this assignment. Part (a) (under Problem Statement) is due after one class period, and parts (b),

(c), (d) and (e) are due after one week. This scheduling allows time for class discussion of these preliminary calculations before the computer program for the stage-to-stage calculations is written.

2. Concepts Demonstrated: The problem illustrates the Lewis-Matheson method of performing the stage-to-stage calculations required for the design of a multicomponent distillation column.

3. Evaluation of Usage: This problem has been used successfully for three years in the junior level separation processes course.

IV. PROGRAM SUMMARY SHEET

V. PROGRAM

1. Program Description: The program performs the stage-to-stage calculations according to the Lewis-Matheson method. The calculations start from assumed product compositions and proceed down the column from the top and up the column from the bottom to the feed plate. If a feed plate match is not achieved, new product compositions are estimated and the calculations are repeated. A feed plate match criteria of 0.0001 mole fraction for each component was chosen.

Important variables in the program include:

Y(I,J)	mole fraction of component i in the vapor leaving stage j
X(I,J)	mole fraction of component i in the liquid leaving stage j
ALPHA(I)	relative volatility of component i
XHK(J)	mole fraction of heavy key component in liquid leaving stage j
YHK(J)	mole fraction of heavy key component in vapor leaving stage j
D	moles of distillate product
B	moles of bottoms product
VR	vapor rate in rectifying section
OR	liquid rate in rectifying section
VS	vapor rate in stripping section
OS	liquid rate in stripping section

R	external reflux ratio
Q	moles of liquid produced on feed plate per mole of feed added
DELD(I)	Correction to moles of distillate for component i

2. Data Input:

a. First Data Card (6I3): Number of components (NCOMP), total number of stages (NTOT), number of stages above feed (NAF), number of stages below feed (NBF), heavy key component (NHK), light key component (NLK).

b. Second - NCOMP Data Cards (3F10.8): Mole fraction in the distillate product (Y(I,1)), mole fraction in the bottoms product (X(I,NTOT)), relative volatility (ALPHA(I)).

c. Last Data Card (8F8.4): Moles of distillate (D), moles of bottoms product (B), vapor rate in rectifying section (VR), liquid rate in rectifying section (OR), vapor rate in stripping section (VS), liquid rate in stripping section (OS), external reflux ratio (R), moles of liquid produced on feed plate per mole of feed added (Q).

3. Output: The results printed out include: the number of stages, the number of stages above the feed, the number of iterations, the liquid and vapor compositions for each component for each stage, moles of each component in the product streams, moles of distillate, moles of bottoms product.

4. Limitations: An arbitrary limit of 10 components and 100 stages is placed on the program. A limit of 100 is placed on the number of iterations.

5. Program Listing:

```
C  MULTICOMPONENT DISTILLATION COLUMN DESIGN
C*****
C      MARCH 13,1972
C*****
C      ORVILLE C. SANDALL
C      DEPARTMENT OF CHEMICAL AND NUCLEAR ENGINEERING
C      UNIVERSITY OF CALIFORNIA, SANTA BARBARA
C*****
C      PLATE TO PLATE CALCULATIONS FOR MULTICOMPONENT DISTILLATION COLUMN
C      DESIGN ASSUMING CONSTANT RELATIVE VOLATILITIES AND CONSTANT MOLAL
C      OVERFLOW
C*****
C      DESCRIPTION OF IMPORTANT VARIABLES:
C
C      NCOMP: NUMBER OF COMPONENTS
C      NTOT: TOTAL NUMBERS OF STAGES
C      NAF: NUMBER OF STAGES ABOVE FEED
C      NBF: NUMBER OF STAGES BELOW FEED
C      NHK: HEAVY KEY COMPONENT
C      NLK: LIGHT KEY COMPONENT
C      Y(I,J): MOLE FRACTION OF COMPONENT I IN VAPOR LEAVING STAGE J
C      X(I,J): MOLE FRACTION OF COMPONENT I IN LIQUID LEAVING STAGE J
C      ALPHA(I): RELATIVE VOLATILITY OF COMPONENT I
C      XHK(J): MOLE FRACTION OF HEAVY KEY COMPONENT IN LIQUID LEAVING
C              STAGE J
C      YHK(J): MOLE FRACTION OF HEAVY KEY COMPONENT IN VAPOR LEAVING
C              STAGE J
C      D: ESTIMATED MOLES OF DISTILLATE PRODUCT
C      B: ESTIMATED MOLES OF BOTTOMS PRODUCT
C      VR: ESTIMATED VAPOR RATE IN RECTIFYING SECTION
C      OR: ESTIMATED LIQUID RATE IN RECTIFYING SECTION
C      VS: ESTIMATED VAPOR RATE IN STRIPPING SECTION
C      OS: ESTIMATED LIQUID RATE IN STRIPPING SECTION
C      R: EXTERNAL REFLUX RATIO
C      Q: MOLES OF LIQUID PRODUCED ON FEED PLATE PER MOLE OF FEED ADDED
C      DELD(I): CORRECTION TO MOLES OF DISTILLATE FOR COMPONENT I
C*****
C      DATA INPUT:
C
C      NCOMP,NTOT,NAF,NBF,NHK,NLK,  6I3
C      Y(I,1),X(I,NTOT),ALPHA(I)  3F10.8
C      D,B,VR,OR,VS,OS,R,Q,  8F8.4
C*****
C      OUTPUT
C
C      THE TOTAL NUMBER OF STAGES
C      THE NUMBER OF STAGES ABOVE FEED
C      NUMBER OF ITERATIONS
C      LIQUID AND VAPOR COMPOSITIONS FOR EACH COMPONENT FOR EACH STAGE
C      MOLES OF EACH COMPONENT IN PRODUCT STREAMS
C      MOLES OF DISTILLATE
C      MOLES OF BOTTOMS PRODUCT
C*****
C      LIMITATIONS
```

```
C
C      A LIMIT OF 10 COMPONENTS AND 100 STAGES IS ARBITRARILY TAKEN
C      A LIMIT OF 100 IS PLACED ON THE NUMBER OF ITERATIONS
C*****
C*****
      DIMENSION Y(10,100),X(10,100),XHK(100),YHK(100),XF(10),A(10),DI(10
     C),BI(10),DELD(10),ALPHA(10)
C READ IN DATA
      READ (5,1) NCOMP,NTOT,NAF,NBF,NHK,NLK
    1 FORMAT (6I3)
      DO 2 J=1,NCOMP
    2 READ (5,3) Y(J,1),X(J,NTOT),ALPHA(J)
    3 FORMAT (3F10.8)
      READ (5,4) D,B,VR,OR,VS,OS,R,Q
    4 FORMAT (8F8.4)
      NF=NAF+1
      NIT=1
    9 I=1
C CALCULATE FROM THE TOP DOWN USING ASSUMED DISTILLATE COMPOSITION
   10 YHK(I)=Y(NHK,I)
      SUM=0.0
      DO 11 J=1,NCOMP
   11 SUM=SUM+Y(J,I)/(ALPHA(J)*YHK(I))
      XHK(I)=1.0/SUM
      DO 12 J=1,NCOMP
   12 X(J,I)=Y(J,I)*XHK(I)/(ALPHA(J)*YHK(I))
      K=I+1
      DO 20 J=1,NCOMP
   20 Y(J,K)=X(J,I)*(R/(R+1.0))+Y(J,1)/(R+1.0)
      IF ( K .GT. NF )  GO TO 100
      I=K
      GO TO 10
  100 CONTINUE
      DO 101 J=1,NCOMP
  101 XF(J)=X(J,NF)
C CALCULATE FROM THE BOTTOM UP USING ASSUMED BOTTOMS COMPOSITION
      M=NTOT
  110 XHK(M)=X(NHK,M)
      SUM=0.0
      DO 111 J=1,NCOMP
  111 SUM=SUM+ALPHA(J)*X(J,M)/XHK(M)
      YHK(M)=1.0/SUM
      DO 112 J=1,NCOMP
  112 Y(J,M)=ALPHA(J)*YHK(M)*X(J,M)/XHK(M)
      L=M-1
      DO 120 J=1,NCOMP
  120 X(J,L)=VS*Y(J,M)/OS+B*X(J,NTOT)/OS
      IF ( L .EQ. NF )  GO TO 200
      M=L
      GO TO 110
  200 CONTINUE
C CHECK TO SEE IF FEED PLATE COMPOSITIONS MATCH
      DO 201 J=1,NCOMP
      A(J)=ABS(XF(J)-X(J,NF))
      IF (A(J) .GT. 0.0001) GO TO 300
  201 CONTINUE
      GO TO 400
  300 CONTINUE
      NIT=NIT+1
      IF(NIT .GT. 100)      GO TO 1000
C ESTIMATE NEW PRODUCT DISTRIBUTION FROM BONNER'S EQUATION
      SD=0.0
      SB=0.0
      DO 301 J=1,NCOMP
      DI(J)=D*Y(J,1)
      BI(J)=B*X(J,NTOT)
      DELD(J)=(X(J,NF)-XF(J))/(XF(J)/DI(J)+X(J,NF)/BI(J))
      DI(J)=DI(J)+DELD(J)
      BI(J)=BI(J)-DELD(J)
      SD=SD+DI(J)
  301 SB=SB+BI(J)
      D=SD
      B=SB
      DO 302 J=1,NCOMP
      Y(J,1)=DI(J)/D
  302 X(J,NTOT)=BI(J)/B
      OS=R*D+Q*100.0
      VS=(R+1.0)*D-(1.0-Q)*100.0
      GO TO 9
C     PRINT OUT RESULTS
  400 WRITE (6,997)
      WRITE ( 6,999)
      WRITE ( 6,999)
      WRITE (6,998)
      WRITE (6,999)
  997 FORMAT (1H1)
  998 FORMAT ( 19H CALCULATED RESULTS )
  999 FORMAT (1H0)
      WRITE (6,398) NTOT
  398 FORMAT ( 1H0,31H  THE TOTAL NUMBER OF STAGES IS,I3)
      WRITE (6,399) NAF
  399 FORMAT ( 1H0,36H  THE NUMBER OF STAGES ABOVE FEED IS,I3)
      WRITE (6,401) NIT
  401 FORMAT ( 1H0,31H  THE NUMBER OF ITERATIONS WERE,I3)
      WRITE (6,402)
  402 FORMAT ( 1H0,78H  STAGE NO.   X1      Y1         X2       Y2
     1X3       Y3          X4       Y4)
      DO 403 N=1,NTOT
  403 WRITE (6,404) N,X(1,N),Y(1,N),X(2,N),Y(2,N),X(3,N),Y(3,N),X(4,N),
     CY(4,N)
  404 FORMAT ( 5H      ,I3,4H     ,F7.5,1H ,F7.5,3H    ,F7.5,1H ,F7.5,3H
     1,F7.5,1H ,F7.5,3H    ,F7.5,1H ,F7.5)
      WRITE (6,410)
  410 FORMAT ( 1H0,29H  COMPONENT    D(I)       B(I))
      DO 411 N=1,NCOMP
  411 WRITE (6,412) N,DI(N),BI(N)
  412 FORMAT (5H     ,I2,6H      ,F7.4,3H   ,F7.4)
      WRITE (6,413)  D
```

```
 413 FORMAT (1H0,30H  THE MOLES OF DISTILLATE ARE ,F8.4)
     WRITE (6,414)  B
 414 FORMAT (1H0,35H  THE MOLES OF BOTTOMS PRODUCT ARE ,F8.4)
     GO TO 1010
1000 WRITE (6,1001)
1001 FORMAT (44H  LIMIT ON NUMBER OF ITERATIONS WAS EXCEEDED)
1010 CONTINUE
     STOP
     END
```

```
CALCULATED RESULTS


   THE TOTAL NUMBER OF STAGES IS 16

   THE NUMBER OF STAGES ABOVE FEED IS  6

   THE NUMBER OF ITERATIONS WERE 13

   STAGE NO.    X1       Y1          X2      Y2          X3      Y3          X4      Y4
       1     0.14056 0.19431     0.67755 0.71868     0.13787 0.06931     0.04402 0.01770
       2     0.10217 0.15430     0.59381 0.68807     0.21913 0.12034     0.08488 0.03729
       3     0.07524 0.12574     0.48799 0.62575     0.29752 0.18081     0.13925 0.06770
       4     0.05719 0.10569     0.38575 0.54699     0.35587 0.23915     0.20119 0.10817
       5     0.04582 0.09226     0.30483 0.47090     0.38597 0.28258     0.26338 0.15427
       6     0.03903 0.08380     0.24928 0.41067     0.39061 0.30498     0.32108 0.20055
       7     0.03505 0.07874     0.21430 0.36933     0.37781 0.30844     0.37284 0.24349
       8     0.02639 0.06077     0.20207 0.35701     0.39068 0.32712     0.38085 0.25511
       9     0.01927 0.04565     0.18463 0.33567     0.40570 0.34957     0.39040 0.26910
      10     0.01358 0.03322     0.16259 0.30523     0.42236 0.37579     0.40147 0.28576
      11     0.00920 0.02330     0.13726 0.26677     0.43954 0.40486     0.41400 0.30507
      12     0.00596 0.01565     0.11049 0.22257     0.45546 0.43483     0.42808 0.32695
      13     0.00368 0.01000     0.08427 0.17585     0.46777 0.46263     0.44428 0.35152
      14     0.00214 0.00602     0.06029 0.13009     0.47336 0.48410     0.46421 0.37980
      15     0.00115 0.00333     0.03964 0.08824     0.46806 0.49385     0.49115 0.41457
      16     0.00054 0.00160     0.02276 0.05221     0.44585 0.48460     0.53084 0.46158

   COMPONENT     C(I)        B(I)
       1        4.9654      0.0400
       2       18.3653      1.6947
       3        1.7711     33.1916
       4        0.4524     39.5186

   THE MOLES OF DISTILLATE ARE  25.5543

   THE MOLES OF BOTTOMS PRODUCT ARE  74.4448
```

I. PROBLEM IDENTIFICATION

1. Title: Multicomponent Distillation Design and Economic Optimization

2. Author: Donald Mackay

3. Affiliation: University of Toronto

II. TECHNICAL DESCRIPTION

1. Problem Statement: Given a multicomponent hydrocarbon feed and required separation specifications design the series of columns (i.e. reflux ratio and number of plates) which will accomplish this separation then cost these to obtain the minimum cost design.

2. Problem Formulation: Each student in the group is set a different problem by selecting different hydrocarbons, different feed compositions, and different separation specifications. A typical example is as follows:

A feed consisting of 1000 lb moles/hr at its bubble point (8500 hr/year) to a distillation column has the molar composition:

n-hexane 25%	3-methylpentane 25%
2-methylpentane 25%	2,2-dimethylbutane 25%

It is to be separated into a distillate containing between 94 and 98% of the most volatile component, the distillate rate being 500 lb moles/hr.

Antoine Constants for these hydrocarbons are available from standard sources, such as API Project 44. Assume ideal liquid and vapour thermodynamic behaviour. Operate at a pressure of 760 mmHg and ignore column pressure drop. Introduce the feed at the middle of the column, do not attempt to optimize feed point location. Assume a vapour velocity of 3 ft/sec. at the top of the column and an overall plate efficiency of 75%.

For design of heat exchangers assume overall heat transfer coefficients of 80 and 100 BTU/ft^2 hr.°F for the boiler and condenser respectively, and log mean ΔT's of 50 and 30°F respectively. Assume a cooling water temperature rise of 40°F. If these assumptions result in non-feasible operating conditions make suitable alterations.

In costing the heat exchangers use a power factor of 0.6 on area and a basic cost of \$12,000 for a 1000 ft^2 boiler and \$9,000 for a 1000 ft^2 condenser.

i.e. cost of boiler of area A ft^2 is $\$12{,}000\ (A/1000)^{0.6}$

Assume a 100 inch diameter plate to cost \$4,000 each with a power factor of 1.5 on diameter.

i.e. cost of plate of diameter D ins. $\$4{,}000\ (D/1000)^{1.5}$

Cooling water costs \$0.05/1000 gal and steam costs \$0.50 per 1000 lb. and assume an enthalpy of vaporization for steam of 920 BTU/lb.

Additional costs (piping instrumentation, insulation etc.) are 75% of cost of column,boiler and condenser.

Annual capital charges are 20% of total costs, i.e. equipment costs and additional costs.

Submit a design report with the following format.

I. Title page.

II. Summary - Brief statement of the problem and the final design ($<$ 100 words).

III. Problem Description - Statement of feed and required separation. Description of components. Cost data used.

IV. Design - Graph of No. of plates vs. Reflux Ratio with actual points given.

Graph of Cost vs. Reflux Ratio with actual points.

Graph of concentration profiles in the column at optimal design.

Description of optimal column design including column diameter and heat exchange areas and cost breakdown, i.e. capital charges and various operating costs. Mass balance.

V. Conclusions and Recommendations. Express your opinion of the project, criticisms and suggestions.

VI. Appendix - Computer outputs for optimal design and two others meeting the specification straddling the optimum.

It should be noted that other costing procedures can be used and other optimization criteria applied, for example, lowest capital cost column.

3. Method of Solution: The following data are read in then printed out. Column Pressure, Lower and Upper temperature limits, number of plates (theoretical), number of the feed plate, number of components, feed and distillate rates, reflux ratio, feed mole fractions, initial guessed distillate mole fractions and Antoine Constants.

A check is made to ensure that the distillate analyses are feasible. The vapour and liquid rates in the rectifying and stripping sections are calculated from the distillate rate, reflux ratio and the feed (liquid at bubble point) rate. The bottoms composition is calculated from an overall mass balance.

The program then calculates by an iterative procedure the actual distillate composition for the specified reflux ratio and number of plates. The student then checks by hand if this column meets the design specifications. If not a suitable adjustment is made to the design.

A plate-to-plate Lewis and Matheson type calculation is started from the top of the column down to the feed plate and is followed by a calculation from the bottom up to the feed plate. If the distillate guess was correct, then the vapour composition leaving the top stripping plate is the same as the vapour composition reaching the bottom rectifying plate. These two compositions will not usually be equal and a mis-match results. The degree of this mis-match is used to estimate the new distillate composition and the computation repeated until a satisfactory match is achieved.

The top-down calculation involves the repeated solution of an equilibrium relationship and a molar balance relationship. The equilibrium relationship involves estimating the composition and temperature of the liquid in equilibrium with a given vapour, i.e. a dew point calculation at known pressure.

This calculation is included as function RECT which calculates $(1-\sum x_i)$ for a given T while subroutine RTMI guesses the next value of T from the previous values of T and the corresponding values of $(1-\Sigma x_i)$. The method used is Mueller's iteration scheme of successive bisection and inverse parabolic interpolation (See G.K. Kristiansen, "Zero of Arbitrary Function", BIT Vol. 3 (1963) pp 205-6.

The calculation of y from x is done by mass balance using the familiar operating line equation. In the case of the bottom up calculation, the procedure is reversed, that is, the composition of vapour in equilibrium with a given liquid is calculated. This again involves bubble point calculation. Function STRIP is used here in which all x_i's are given and $(1-\Sigma y_i)$ is calculated. RTMI is used to calculate a new T as before. The mass balance equation involves the calculation of x from y using the stripping operating line equation.

The next mathematical problem is the re-estimation of the distillate composition based on the mis-match. The method used in this case is a modified Theta method. It should be noted that the estimation of Theta on each occasion is in itself an iterative procedure and requires a special subroutine which is in this case Newton's method.

The mathematical basis of the theta method is that each new component distillate rate d_i (moles/hr) is calculated from

$$d_{i\,NEW} = f_i \Big/ \left\{ 1 + \theta \left[\frac{b_i}{d_i} \cdot \frac{V_{iR}}{V_{iS}} \right]_{OLD} \right\}$$

where f_i is the feed rate of i, b_i is the old bottoms rate and V_{iR} and V_{iS} are the vapour rates of i at the feed plate as calculated from the top-down (rectifying) and bottom-up (stripping) plate to plate calculations. θ is determined such that its value satisfies the criterion that the sum of the individual new distillate rates $d_{i\,NEW}$ is the required total distillate rate. As the values of d_i approach the correct value V_{iR} approaches V_{iS} and θ approaches unity.

When the mis-match at the feed plate is small enough the program stops iterating and prints out the results. The criterion used here is that the sum of squares of the mis-matches should be less than a predetermined tolerance. In this case the root mean square deviation RMS is calculated at each iteration (and printed out) and when this is sufficiently small the program is terminated

$$\mathrm{RMS} = \sqrt{\sum_{i} (\Delta y)^2/(\mathrm{N}^{\mathrm{o}} \text{ of components})}$$

where Δy is the difference between top-down and bottom-up calculated vapour compositions at the feed point.

A separate print out subroutine is included (SCRIBE) which prints out the column profiles after the first and last iteration.

Subroutine EXT is used in case of emergency.

The general procedure is to locate the combinations of reflux ratio and number of plates which meet the required separation specifications. This is best done on a graph of these variables in which three areas are located, one of better-than-required separation, one of inadequate separation and a band between of acceptable separations.

The mid-point locus of this band gives a series of acceptable columns each of which is costed separately to determine the minimum cost column. This can be done by hand calculation or by a program written by the student.

4. References: A description of the theta method can be found in "Multicomponent Distillation" by C.D. Holland, Prentice-Hall, (1963).

Antoine Constants for hydrocarbon vapour pressures can be obtained from publications arising from the API Project 44.

Cost data and costing techniques can be found in "Plant Design and Economics for Chemical Engineers" by M.S. Peters and K.D. Timmerhaus, McGraw-Hill, (1968).

5. Solution: A typical program output is shown. Also given are typical graphs of Reflux Ratios vs. number of plates and costs. These are self explanatory.

III. EDUCATIONAL (PEDAGOGICAL) ASPECTS

1. Description of Past Usage: This project has been used successfully for three years for final year students taking a course in advanced separation processes which includes multicomponent distillation material.

2. Concepts Demonstrated: The project teaches the design of multicomponent distillation columns using a plate-to-plate method. This is a logical extension to previous work on graphical McCabe-Thiele construction and gives a valuable insight into multicomponent computation. It brings to the student the essential differences between design and simulation of distillation columns. It illustrates clearly that the required separation can be achieved by a number of columns which represent combinations of numbers of plates and reflux ratios. By costing a number of designs the student obtains an optimum (lowest cost) and thus obtains experience in practical costing. Hopefully the project sharpens his skills in computer programming, costing, thermodynamics of equilibrium, elementary design and multicomponent mass transfer operations. Probably its main advantage is that it integrates all these topics in one project and clearly demonstrates the connection between these topics hitherto treated in separate courses.

3. Evaluation of Usage: Students usually are allowed about 4 weeks to complete the project. They are encouraged to modify the program, possibly to run a series of designs.

4. Nature of Assignment: Each student is set a different problem and is required to produce an individual report. He is given the basic deck of cards. Advice on programming and distillation is made available.

IV. PROGRAM SUMMARY SHEET

V. PROGRAM DESCRIPTION

1. General Description: The program can be divided into a number of sections, data input and output and a column mass balance. This is followed by a top-down plate-to-plate computation which are alternate equilibrium and mass balance calculations. After a similar bottom-up calculation the mis-match at the feed is examined and used to guess a new distillate composition employing the theta method. The computation is repeated until the mis-match is satisfactorily small.

2. External Description: The logic is straightforward and should be easily followed with the aid of comment cards.

```
C*******************************************************************************
C*******************************************************************************
C                                                                             **
C                                                                             **
C          DATA INPUT                                                         **
C                                                                             **
C                                                                             **
C  P IS THE COLUMN PRESSURE IN MM. OF MERCURY                                 **
C  TL  IS THE LOWER TEMPERATURE LIMIT IN DEGREES CENTIGRADE                   **
C  TU  IS THE UPPER TEMPERATURE LIMIT IN DEGREES CENTIGRADE                   **
C  NPLTS  IS THE NUMBER OF PLATES IN THE COLUMN                               **
C  NF  IS THE NUMBER OF THE FEED PLATE                                        **
C  NCCMP  IS THE NUMBER OF COMPONENTS                                         **
C   F  IS THE FEED RATE IN MOLES/HOUR                                         **
C   D  IS THE DISTILLATE RATE IN MOLES/HOUR                                   **
C    R  IS THE REFLUX RAT IO                                                  **
C  XF(I)  IS THE LIQUID MOLE FRACTION OF COMPONENT I IN THE FEED              **
C  XD(I)  IS THE LIQUID MOLE FRACTION OF COMPONENT I IN THE DISTILLATE        **
C  A(I) IS THE A IN ANTCINES EQUATION FOR COMPONENT I                         **
C  AB(I)  IS THE B IN ANTOINES EQUATION FOR COMPONENT I                       **
C  AC(I)  IS THE C IN ANTOINES EQUATION FOR COMPONENT I                       **
C                                                                             **
C                                                                             **
C  NRUNS  IS THE NUMBER OF RUNS WITH DIFFERENT F.D.AND R                      **
C                                                                             **
C                                                                             **
C*******************************************************************************
C*******************************************************************************
```

```
      CCMMCN P.NCOMP.NPLTS.NF.N.  A(6).AB(6).AC(6).XF(6)
      COMMCN XR(41.6).YR(41.6).TR(41).XS(41.6).YS(41.6).TS(41)
      DIMENSIONBDC(6).FXF(6).XD(6).DXD(6).XB(6).BXB(6).RR(6).RS(6).DC(6)
      REAL LR.LS
      EXTERNAL RECT.STRIP.EXT
      WRITE(6.4)
    4 FCRMAT(1H1)
      READ(5.666) P.TL.TU
  666 FORMAT(3F11.5)
    1 READ(5.101)NPLTS.NF.NCCMP
  101 FORMAT(3I3)
    2 READ(5.667) (XF(I). I=1.NCOMP)
      READ(5.667) (XD(I). I=1.NCOMP)
  667 FORMAT(8F10.7)
      READ(5.103) (A(I).AB(I).AC(I). I=1.NCOMP)
  103 FORMAT(3F11.5)
      READ(5.101)NRUNS
      DC 69 IJK=1.NRUNS
      READ(5.102) F.D.R
  102 FORMAT(8F10.4)
```

```
C***************************************************************************
C***************************************************************************
C                                                                         **
C                                                                         **
C   MASS BALANCES ON DISTILLATE AND FEED                                  **
C                                                                         **
C                                                                         **
C    DXD(I) IS THE DISTILLATE RATE OF COMPONENT I IN MOLES/HOUR           **
C    FXF(I) IS THE FEED RATE OF COMPONENT I IN MOLES/HOUR                 **
C  S    IS USED TO CHECK IF THE LIQUID MOLE FRACTION OF I IN THE FEED IS GREATER*
C  THAN UNITY                                                             **

C   SD  IS USED TO CHECK IF THE LIQUID MOLE FRACTION OF I IN THE DISTILLATE IS**
C  GREATER THAN UNITY                                                     **
C                                                                         **
C                                                                         **
C***************************************************************************
C***************************************************************************
        S=0.
        SD=0.
        DO  3    I= 1.NCOMP
        DXD(I) = XD(I) *D
        FXF(I)=F*XF(I)
        IF(DXD(I) .GT.FXF(I)  ) CALL EXT(5)                            ** EXIT
        S = S+ XF(I)
        SD = SD+XD(I)
  3     CONTINUE
        IF(ABS(S-1.0) .GT. 1.E-5 .OR. ABS(SD-1.0).GT. 1.E-5)CALL EXT(4)   ** EXIT
C***************************************************************************
```

```
C***********************************************************************
C                                                                     **
C                                                                     **
C         DATA OUTPUT                                                 **
C                                                                     **
C                                                                     **
C***********************************************************************
C***********************************************************************
      WRITE(6,305)R,F,D
  305 FCRMAT(1X,13HREFLUX RATIO=,F5.2,2X,21HFEED RATE(MOLE/HCUR)= ,
     1F8.2,5X,29HDISTILLATE RATE (MOLES/HOUR)=,F8.2//)
      WRITE(6,306) (XF(I), I =1,NCOMP )
  306 FORMAT(1X,17HFEED COMPCSITION=,8F8.3//)
      WRITE(6,307) (XD(I),I=1,NCOMP)
  307 FCRMAT(1X,32HDISTILLATE COMPOSITION(INITIAL)=,8F8.3//)
      WRITE(6,60)
   60 FCRMAT(2X,17HANTOINE CCNSTANTS,3X,1HA,10X,1HB,11X,1HC/)
      DC 61 I=1,NCCMP
      WRITE(6,80) A(I),AB(I),AC(I)
   80 FORMAT(15X,F11.5,1X,F11.5,1X,F11.5/)
   61 CCNTINUE
      WRITE(6,130)TL,TU
  130 FORMAT(2X,18HTEMPERATURE LIMITS,2F8.2,18H DEGREE CENTIGRADE//)
      WRITE(6,110)P
  110 FORMAT(2X,9HPRESSLRE=,F10.1 ,10H MM. OF HG   )
      WRITE(6,140)
  140 FORMAT(1H0)
```

```
C****************************************************************************
C****************************************************************************
C                                                                          **
C                                                                          **
C    VAPOUR AND LIQUID MCLAR FLOW RATES                                    **
C                                                                          **
C                                                                          **
C   VO  IS THE VAPOUR RATE IN THE COLUMN IN MOLES/HOUR                     **
C   VS IS THE VAPOUR RATE IN THE STRIPPING SECTION IN MOLES/HOUR           **
C   VR  IS THE VAPOUR RATE IN THE RECTIFYING SECTION IN MOLES/HOUR         **
C   LS  IS THE LIQUID RATE IN THE STRIPPING SECTION IN MOLES/HOUR          **
C   LR  IS THE LIQUID RATE IN THE RECTIFYING SECTION IN MOLES/HOUR         **
C   THTA  IS THE THETA USED IN THE THETA METHOD                            **
C                                                                          **
C                                                                          **
C****************************************************************************



C****************************************************************************
      VC=D*(R+1.0)
      B = F-D
      VR=VC
      VS=VC
      LR =VC-D
      LS =LR+F
      THTA=0.0
      NP1=NPLTS+1
```

```
C*******************************************************************************
C*******************************************************************************
C                                                                             **
C                                                                             **
C     RECTIFYING SECTION. INITIAL CALCULATIONS                                **
C                                                                             **
C                                                                             **
C  YR(N,I)  IS THE VAPOUR MOLE FRACTION OF COMPONENT I ON PLATE N IN THE      **
C RECTIFYING SECTION.  SUBROUTINE RTMI ALONG WITH SUBROUTINE RECT, CALCULATES **
C XR(N,I),(THE LIQUID MOLE FRACTION OF COMPONENT I), IN EQUILIBRIUM WITH ITS  **
C VAPOUR YR(N,I) ON PLATE N.  THE TEMPERATURE ON EACH PLATE IS ALSO CALCULATED**
C  SIMULTANEOUSLY ALONG WITH XR AND YR.                                       **
C                                                                             **
C                                                                             **
C*******************************************************************************
C*******************************************************************************
   10   DO 24 J =1,25
        SUMF=0.0
        N = NF1
        DO 11 I =1,NCOMP
   11   YR(N,I) = DXD(I)/C
  111   CONTINUE
        CALL RTMI (TR(N),FT,RECT,TL,TU,0.0001,50,L)
        IF(N.EQ.NF) GO TO 14
        N = N-1
```

```
C***********************************************************************
C***********************************************************************
C                                                                     **
C                                                                     **
C              STANDARD MASS BALANCE FOR RECTIFYING SECTION           **
C                                                                     **
C                                                                     **
C  THIS CALCULATES YR(N,I) FROM THE LIQUID COMPOSITION XR(N+1,I)      **
C                                                                     **
C                                                                     **
C***********************************************************************
C***********************************************************************
      DO 13 I =1,NCOMP
   13 YR(N,I) = (LR/VR)*XR(N+1,I)+DXD(I)/VR
      GO TO 111
   14 CONTINUE
C***********************************************************************
C***********************************************************************
C                                                                     **
C                                                                     **
C     CALCULATION OF RR                                               **
C                                                                     **
C                                                                     **
C      RR(I)  IS USED IN DETERMINING THE RATIO OF B(I) TO D(I)        **
C                                                                     **
C                                                                     **
C***********************************************************************
C***********************************************************************
      DO 15 I =1,NCOMP
   15 RR(I) = VR*YR(NF,I)/DXD(I)
```

```
C*****************************************************************************
C*****************************************************************************
C                                                                           **
C                                                                           **
C        STRIPPING SECTION, INITIAL CALCULATIONS                            **
C                                                                           **
C                                                                           **
C     SUBRCUTINE RTMI ALONG WITH SUBROUTINE STRIP CALCULATES YS(N,I), WHICH IS**
C THE VAPOUR MOLE FRACTION OF COMPONENT I IN EQUILIBRIUM WITH ITS LICUID XS(N,I)
C CN PLATE N. THE TEMPERATURE IS ALSO CALCULATED SIMULTANEOUSLY ALONG WITH XS **
C AND YS.                                                                   **
C                                                                           **
C                                                                           **
C*****************************************************************************
C*****************************************************************************
          N = 1
          DC 16 I =1,NCOMP
          BXB(I) =FXF(I)-DXD(I)
   16     XS(N,I) =BXB(I)/B
   17     CCNTINUE
          CALL RTMI (TS(N),FT,STRIP,TL,TU,0.0001,50,L)
  170     IF(N.EQ.NF) GO TO 185
          N = N+1
C*****************************************************************************
C*****************************************************************************
C                                                                           **
C                                                                           **
C        STANDARD MASS BALANCE FOR STRIPPING SECTION                        **
C                                                                           **
C                                                                           **
C   THIS CALCULATES XS(N,I) FROM THE VAPOUR COMPOSITICN, YS(N-1,I).
C                                                                           **
C                                                                           **
C*****************************************************************************
C*****************************************************************************
```

```
      DC 18 I =1,NCOMP
   18 XS(N,I) =(VS/LS)*YS(N-1,I)+BXB(I)/LS
      GO TC 17
C***********************************************************************
C***********************************************************************
C                                                                     **
C                                                                     **
C       FIRST ITERATION PRINTCUT CONCENTRATIONS                       **
C                                                                     **
C    THIS SHCWS THE DEGREE OF THE MISMATCH AT THE FEED PLATE          **
C  BDC(I) , WHICH IS THE RATIO OF RR(I) TO RS(I), GIVES THE RATIO OF B(I)/D(I)**
C  DC(I)  IS THE NEW DISTILLATE RATE OF COMPONENT I, IN MCLES/HOUR    **
C                                                                     **
C                                                                     **
C***********************************************************************
C***********************************************************************
  185 IF(J.EQ.1) WRITE(6,112)
      CALL SCRIBE(J       )
      WRITE(6,118) NF, TR(NF), TS(NF)
  118 FORMAT(//10X, 15HAT FEED PLATE  ,I2,5X,33H THE MISMATCHED TEMPERAT
     1URES ARE ,F8.3,2X,F8.3)




   19 CONTINUE
      DC 20 I =1,NCOMP
      RS(I) = VS*YS(NF,I) /BXB(I)
      BDC(I) =RR(I)/RS(I)
      DC(I) =FXF(I)/(BDC(I)+1.)
   20 SUMF =SUMF+DC(I)
```

```
C******************************************************************************
C******************************************************************************
C                                                                            **
C                                                                            **
C               THETA ITERATIVE ROUTINE  (NEWTCN METHOD)                     **
C                                                                            **
C    THE TCLERANCE (TOL) USEC IN THE THETA METHOD IS 0.0001                  **
C                                                                            **
C                                                                            **
C******************************************************************************
C******************************************************************************
   21    ST1 = 0.
         STH = 0.
         DC 22 I =1.NCOMP
         SGTH =FXF(I)/(1.0+(THTA*BDC(I)))
         STH = STH+SGTH
         SGT1 =SGTH*SGTH*BCC(I)/FXF(I)
   22    ST1 = ST1-SGT1
         CHANGE = ((STH-D)/ST1)
         THNEW =THTA-CHANGE
         TCL = .0001*THTA
         TEST =ABS(CHANGE)
         THTA=THNEW
         WRITE(6.122) THTA
  122    FCRMAT(10X.8HTHETA = .F8.5)
         IF(TEST.GT. TOL ) GO TO 21
         DC 23 I =1.NCCMP
```

```
C***************************************************************************
C***************************************************************************
C                                                                         **
C                                                                         **
C        NEW DISTILLATE COMPOSITION                                       **
C                                                                         **
C   THIS CALCULATES A NEW DISTILLATE RATE AND A NEW DISTILLATE COMPOSITION **
C  FOR COMPONENT I, WHICH IS BASED ON THE NEW VALUE FOR THETA             **
C                                                                         **
C                                                                         **
C***************************************************************************
C***************************************************************************
      DXD(I) =FXF(I)/(1.0+(THTA*BDC(I)))
   23 XD(I) = DXD(I) /D
      WRITE(6,120) (XD(I),I=1,NCOMP)
  120 FORMAT(37H DISTILLATE COMPOSITION(ITERATIVE) = ,8F8.3)
C***************************************************************************
C***************************************************************************
C                                                                         **
C                                                                         **
C                      DISTILLATE CONVERGENCE ROUTINE                     **
C                                                                         **
C          ROOT MEAN SQUARE DEVIATION OF YR-YS AT THE FEED PLATE          **
C                                                                         **
C      IF THE RMS DEVIATION IS LESS THAN 0.005, CONVERGENCE HAS BEEN REACHED **
C  AND THE CONCENTRATION PROFILE IS PRINTED OUT                           **
C                                                                         **
C                                                                         **
C***************************************************************************
C***************************************************************************
```

```
      SUMSQ = 0.0
      DO 231 I = 1,NCOMP
      SUMSQ = SUMSQ+(YR(NF,I)-YS(NF,I) )**2
  231 CONTINUE
      RMS = SQRT(SUMSQ/NCOMP)
      WRITE(6,68)RMS
   68 FORMAT(40H THE RMS DEVIATION AT THE FEED PLATE IS ,F12.6)
      IF(RMS .LT. 0.005 ) GO TO 25
   24 CONTINUE
      CALL EXT(25)                                                    ** EXIT
    25 DO 26 I = 1,NCOMP
      XD(I) =YR(NP1,I)
   26 XB(I) =XS(1,I)
C*************************************************************************
C*************************************************************************
C                                                                       **
C                                                                       **
C                           END OF CALCULATIONS                         **
C                               PRINTOUT                                **
C                                                                       **
C                                                                       **
C*************************************************************************
C*************************************************************************
      WRITE(6,112)
    112 FORMAT(////10X,1HN,4X,1HT,6X,4HY(1),5X,4HX(1),5X,4HY(2),5X,4HX(2),
     1 5X,4HY(3),5X,4HX(3),5X,4HY(4),5X,4HX(4),5X,4HY(5),5X,4HX(5),
     2 5X,4HY(6),5X,4HX(6))
      WRITE(6,149) (XD(I) ,I = 1,NCOMP )
  149 FORMAT(11H DISTILLATE,10X,6(9X,F7.5,2X))
      CALL SCRIBE(0)
      WRITE(6,152) (XB(I) ,I =1,NCOMP )
  152 FORMAT(9H  BOTTOMS  ,12X,6(9X,F7.5,2X),/)
      WRITE(6,153)
  153 FORMAT(1H1)
    69 CONTINUE
      STOP
      END                                                           PROGRAM
```

```
C*****************************************************************************
C*****************************************************************************
C                                                                           **
C                                                                           **
C                                   FUNCTION RECT(T)                        **
C                                                                           **
C         THIS FUNCTION PERFORMS A DEW POINT CALCULATION. GIVEN P, YR(N,I), AND**
C   T FRCM SUBROUTINE RTMI, IT CALCULATES THE LIQUID MOLE FRACTION XR(N,I) IN  **
C   THE RECTIFYING SECTICN                                                  **
C                                                                           **
C                                                                           **
C*****************************************************************************
C*****************************************************************************
      FUNCTICN RECT(T)
      COMMCN P,NCOMP,NPLTS,NF,N,  A(6),AB(6),AC(6),XF(6)
      CCMMCN XR(41,6),YR(41,6),TR(41),XS(41,6),YS(41,6),TS(41)
      SUM = 0.0
      DC 1 I = 1,NCOMP
      XR(N,I) =(P*YR(N,I))/(EXP(2.3026*(A(I)-(AB(I)/(T+AC(I))))))




    1 SUM = SUM+ XR(N,I)
      RECT= 1.-SUM
      RETURN
      END
```

```
C*********************************************************************************
C*********************************************************************************
C                                                                              **
C                                                                              **
C                           FUNCTION STRIP(T)                                  **
C                                                                              **
C         THIS FUNCTION PERFORMS A BUBBLE POINT CALCULATION. GIVEN P. XS(N.I).  **
C   IT CALCULATES THE VAPOUR MOLE FRACTION YS(N.I) IN THE STRIPPING SECTION    **
C                                                                              **
C                                                                              **
C*********************************************************************************
C*********************************************************************************

      FUNCTICN STRIP(T)
      COMMCN P.NCOMP.NPLTS.NF.N.  A(6).AB(6).AC(6).XF(6)
      CCMMCN XR(41.6).YR(41.6).TR(41).XS(41.6).YS(41.6).TS(41)
      SUM = 0.0
      DC 1 I = 1.NCOMP
      YS(N.I) =EXP(2.3026*(A(I)-AB(I)/(T+AC(I))))  *XS(N.I)/P
    1 SUM = SUM+YS(N,I)
      STRIF = 1. - SUM
      RETURN
      END
```

```
C*******************************************************************************
C*******************************************************************************
C                                                                             **
C                                                                             **
C                          SUBROUTINE EXT(NNNN)                               **
C                                                                             **
C      THIS SUBROUTINE IS USEDIN CASE OF EMERGENCY. IF ANYTHING GOES WRCNG.   **
C  EXIT PCRTS THRCUGHOUT THE PROGRAM WILL BE PRINTED OUT AND THE PROBLEM     **
C  LOCATED CUICKLY                                                            **
C                                                                             **
C                                                                             **
C*******************************************************************************
C*******************************************************************************

      SUBRCUTINE EXT ( NNNN )                                          ** EXIT
      WRITE(6,111) NNNN
  111 FCRMAT(12H STOP ***** ,I3,6H ***** )
      CALL EXIT
      RETURN
      END
```

```
C*******************************************************************************
C*******************************************************************************
C                                                                             **
C                                                                             **
C                         SUBROUTINE RTMI                                     **
C                                                                             **
C      THIS SUBROUTINE CETERMINES THE ROOTS. TR(N). AND TS(N). OF THE EQUATIONS*
C  USED IN FUNCTIONS RECT(T) AND STRIP(T) RESPECTIVELY. IT USES THE EQUATIONS **
C  FOR XR(N.I) AND YS(N.I) TC CALCULATE THE CORRESPONDING T. IT ITERATES WITH **
C  A TOLERANCE (EPS) OF 0.0001 UNTIL.                                         **
C                        1.0 - SIGMAXR(N.I)   0.0001  AND.                    **
C                        1.0 - SIGMAYS(N.I)   0.0001                          **
C      THUS A TEMPERATURE IS CHOSEN. MUELLER'S ITERATION SCHEME OF SUCCESSIVE **
C  BISECTICN AND INVERSE PARABOLIC INTERPRETATION IS USED                     **
C                                                                             **
C                                                                             **
C   NCTE.  X  IS THE TEMPERATURE TR(N). OR TS(N).                             **
C          F  IS A FUNCTICN CF TEMPERATURE.                                   **
C          FCT  IS FUNCTION RECT(T) OR STRIP(T).                              **
C          XLI  IS TL                                                         **
C          XRI  IS TU                                                         **
C          EPS  IS THE TOLERANCE                                              **
C          IEND  IS THE NUMBER OF ITERATIONS                                  **
C          IER IS A REFERENCE WHICH TELLS THE PROGRAMMER WHICH PART CF RTMI   **
C            HAS BEEN USED                                                    **
C                                                                             **
C                                                                             **
C*******************************************************************************
C*******************************************************************************
```

```
      SUBRCUTINE RTMI(X,F,FCT,XLI,XRI,EPS,IEND,IER)                     RTMI 560
      EXTERNAL RECT,STRIP,EXT                                           ** TOLSE
      IER=0                                                             RTMI 600
      XL=XLI                                                            RTMI 610
      XR=XRI                                                            RTMI 620
      X=XL                                                              RTMI 630
      TOL=X                                                             RTMI 640
      F=FCT(TOL)                                                        RTMI 650
      IF(F)1,16,1                                                       RTMI 660
    1 FL=F                                                              RTMI 670
      X=XR                                                              RTMI 680
      TCL=X                                                             RTMI 690
      F=FCT(TOL)                                                        RTMI 700
      IF(F)2,16,2                                                       RTMI 710
    2 FR=F                                                              RTMI 720
      IF(FL*FR ) 3,25,25                                                ** IF
    3 I=0                                                               RTMI 770
      TOLF=EPS
    4 I=I+1                                                             RTMI 820
      DO 13 K=1,IEND                                                    RTMI 850
      X=.5*(XL+XR)                                                      RTMI 860
      TCL=X                                                             RTMI 870
      F=FCT(TOL)                                                        RTMI 880
      IF(F)5,16,5                                                       RTMI 890
5     IF( F*FR ) 6,7,7                                                  ** IF
    6 TCL=XL                                                            RTMI 930
      XL=XR                                                             RTMI 940
      XR=TCL                                                            RTMI 950
      TOL=FL                                                            RTMI 960
      FL=FR                                                             RTMI 970
      FR=TCL                                                            RTMI 980
    7 TCL=F-FL                                                          RTMI 990
      A=F*TCL                                                           RTMI1000
      A=A+A                                                             RTMI1010
      IF(A-FR*(FR-FL))8,9,9                                             RTMI1020
    8 IF(I-IEND)17,17,9                                                  RTMI1030
    9 XR=X                                                               RTMI1040
      FR=F                                                               RTMI1050
      TOL=EPS                                                            RTMI1080
      A=ABS(XR)                                                          RTMI1090
      IF(A-1.)11,11,10                                                   RTMI1100
   10 TOL=TOL*A                                                          RTMI1110
   11 IF(ABS(XR-XL)-TOL)12,12,13                                         RTMI1120
```

```
   12 IF(ABS(FR-FL)-TOLF)14,14,13                                        RTMI1130
   13 CONTINUE                                                           RTMI1140
      IER=1                                                              RTMI1200
      WRITE(6,111) X,F                                                   **
  111 FORMAT(2X,2E14.5)
  131 CALL EXT(10)                                                       ** EXIT
   14 IF(ABS(FR)-ABS(FL))16,16,15                                        RTMI1210
   15 X=XL                                                               RTMI1220
      F=FL                                                               RTMI1230
      WRITE(6, 111) X,F
   16 RETURN                                                             **RETURN
   17 A=FR-F                                                             RTMI1270
      DX=(X-XL)*FL*(1.+F*(A-TOL)/(A*(FR-FL)))/TOL                        RTMI1280
      XM=X                                                               RTMI1290
      FM=F                                                               RTMI1300
      X=XL-DX                                                            RTMI1310
      TOL=X                                                              RTMI1320
      F=FCT(TOL)                                                        RTMI1330
      IF(F)18,16,18                                                     RTMI1340
   18 TOL=EPS                                                           RTMI1370
      A=ABS(X)                                                          RTMI1380
      IF(A-1.)20,20,19                                                  RTMI1390
   19 TCL=TCL*A                                                         RTMI1400
   20 IF(ABS(DX)-TOL)21,21,22                                           RTMI1410
   21 IF(ABS(F)-TOLF)16,16,22                                           RTMI1420
 22   IF( F*FL ) 23,24,24                                               ** IF
   23 XR=X                                                              RTMI1460
      FR=F                                                              RTMI1470
      GC TC 4                                                           RTMI1480
   24 XL=X                                                              RTMI1490
      FL=F                                                              RTMI1500
      XR=XM                                                             RTMI1510
      FR=FM                                                             RTMI1520
      GC TC 4                                                           RTMI1530
   25 IER=2                                                             RTMI1580
 26   CALL EXT(20)                                                      ** EXIT
      RETURN                                                            RTMI1590
      END                                                               RTMI1600
C***********************************************************************************
```

```
C********************************************************************************
C                                                                              **
C                                                                              **
C                        SUBROUTINE SCRIBE(JJ)                                 **
C                                                                              **
C      THIS IS A PRINTOUT SUBROUTINE WHICH PRINTS OUT THE COLUMN CONCENTRATION**
C  PROFILES AFTER THE FIRST AND LAST ITERATION                                 **
C                                                                              **
C                                                                              **
C********************************************************************************
C********************************************************************************

      SUBRCUTINE SCRIBE (JJ)
      CCMMCN P,NCOMP,NPLTS,NF,N,  A(6),AB(6),AC(6),XF(6)
      COMMCN XR(41,6),YR(41,6),TR(41),XS(41,6),YS(41,6),TS(41)
      IF(JJ.NE.0.AND.JJ.NE.1 ) RETURN
      NP1 = NPLTS +1
      DC 50III = 1,NP1
      NI = NP1+1-III
   40 IF(NI.GE.NF) WRITE(6,150) NI,TR(NI),(YR(NI,I),XR(NI,I),I=1,NCOMP)
   41 IF(NI.EQ.NF) WRITE(6,151)            (XF(I),I =1,NCOMP)

   42 IF(NI.LE.NF) WRITE(6,150) NI,TS(NI),(YS(NI,I),XS(NI,I),I =1,NCCMP)
   50 CONTINUE
  150 FORMAT(10X,I2,1X,F7.3,1X,12(F7.5,2X),1X )
  151 FORMAT(5H FEED,16X,6(9X,F7.5,2X))
      IF(JJ.EQ.0 ) RETURN
      RETURN
      END
```

```
REFLUX RATIO= 3.00  FEED RATE(MOLE/HOUR)= 1000.00      DISTILLATE RATE (MOLES/HOUR)=  500.00


FEED COMPOSITION=   0.250   0.250   0.250   0.250
DISTILLATE COMPOSITION(INITIAL)=   0.250   0.250   0.250   0.250
 ANTOINE CONSTANTS    A           B           C

                   6.87776  1171.53000   224.36590

                   6.83910  1135.40900   226.57200

                   6.84887  1152.36700   227.12890

                   6.75483  1081.17600   229.34300

 TEMPERATURE LIMITS    0.00  300.00 DEGREE CENTIGRADE


 PRESSURE=     760.0 MM. OF HG
```

```
           N     T      Y(1)      X(1)      Y(2)      X(2)      Y(3)      X(3)      Y(4)      X(4)
          21  61.338 0.25000   0.31731   0.25000   0.24169   0.25000   0.26587   0.25000   0.17513
          20  62.309 0.30048   0.36938   0.24377   0.22859   0.26190   0.27006   0.19385   0.13198
          19  62.933 0.33953   0.40894   0.23394   0.21513   0.26505   0.26797   0.16148   0.10796
          18  63.335 0.36921   0.43888   0.22385   0.20329   0.26348   0.26303   0.14347   0.09480
          17  63.599 0.39166   0.46158   0.21497   0.19363   0.25977   0.25719   0.13360   0.08760
          16  63.778 0.40869   0.47887   0.20772   0.18607   0.25539   0.25144   0.12820   0.08363
          15  63.901 0.42165   0.49208   0.20205   0.18029   0.25108   0.24623   0.12522   0.08139
          14  63.989 0.43156   0.50220   0.19772   0.17595   0.24718   0.24174   0.12355   0.08010
          13  64.053 0.43915   0.50998   0.19446   0.17271   0.24381   0.23797   0.12258   0.07933
          12  64.100 0.44499   0.51598   0.19204   0.17031   0.24098   0.23487   0.12199   0.07884
          11  64.135 0.44949   0.52060   0.19023   0.16853   0.23865   0.23234   0.12163   0.07853
          10  64.161 0.45295   0.52417   0.18890   0.16721   0.23676   0.23031   0.12140   0.07832
FEED                           0.25000             0.25000             0.25000             0.25000
          10  54.540 0.06399   0.10223   0.13424   0.16165   0.09964   0.13231   0.70212   0.60380
           9  54.675 0.06529   0.10383   0.13957   0.16732   0.10288   0.13600   0.69226   0.59286
           8  54.863 0.06728   0.10630   0.14665   0.17471   0.10750   0.14120   0.67858   0.57778
           7  55.125 0.07038   0.11019   0.15589   0.18413   0.11400   0.14845   0.65973   0.55722
           6  55.485 0.07524   0.11634   0.16767   0.19570   0.12307   0.15834   0.63403   0.52961
           5  55.977 0.08292   0.12608   0.18213   0.20919   0.13543   0.17143   0.59952   0.49330
           4  56.633 0.09510   0.14137   0.19898   0.22370   0.15179   0.18802   0.55413   0.44692
           3  57.488 0.11421   0.16492   0.21712   0.23740   0.17252   0.20778   0.49615   0.38991
           2  58.563 0.14365   0.20001   0.23425   0.24739   0.19722   0.22935   0.42488   0.32325
           1  59.857 0.18752   0.25000   0.24673   0.25000   0.22418   0.25000   0.34156   0.25000
          AT FEED PLATE  10       THE MISMATCHED TEMPERATURES ARE   64.161     54.540
          THETA =  0.18125
          THETA =  0.43396
          THETA =  0.60448
          THETA =  0.64230
          THETA =  0.64360
          THETA =  0.64360
DISTILLATE COMPOSITICN(ITERATIVE) =     0.090   0.262   0.198   0.450




THE RMS DEVIATION AT THE FEED PLATE IS     0.357181


          AT FEED PLATE  10       THE MISMATCHED TEMPERATURES ARE   61.672     58.755
          THETA =  0.83546
          THETA =  0.86867
          THETA =  0.86941
          THETA =  0.86941
DISTILLATE COMPOSITICN(ITERATIVE) =     0.061   0.277   0.188   0.474
THE RMS DEVIATION AT THE FEED PLATE IS     0.110511
```

```
        AT FEED PLATE  10      THE MISMATCHED TEMPERATURES ARE   61.000    60.336
        THETA =  0.96781
        THETA =  0.97413
        THETA =  0.97415
DISTILLATE COMPOSITICN(ITERATIVE) =    0.055   0.282   0.186   0.478
THE RMS DEVIATION AT THE FEED PLATE IS      0.025253

        AT FEED PLATE  10      THE MISMATCHED TEMPERATURES ARE   60.827    60.689
        THETA =  0.99472
        THETA =  0.99496
        THETA =  0.99496
DISTILLATE COMPOSITICN(ITERATIVE) =    0.053   0.283   0.186   0.478
THE RMS DEVIATION AT THE FEED PLATE IS      0.005284

        AT FEED PLATE  10      THE MISMATCHED TEMPERATURES ARE   60.789    60.761
        THETA =  0.99897
        THETA =  0.99898
DISTILLATE CCMPOSITICN(ITERATIVE) =    0.053   0.283   0.185   0.479
THE RMS DEVIATION AT THE FEED PLATE IS      0.001089
```

```
               N       T      Y(1)       X(1)       Y(2)       X(2)       Y(3)       X(3)       Y(4)       X(4)
DISTILLATE                          0.05340               0.28269               0.18552               0.47839
              21  57.032 0.05340  0.07831    0.28269    0.31370    0.18552    0.22681    0.47839    0.38118
              20  58.047 0.07208  0.10213    0.30595    0.32853    0.21649    0.25602    0.40548    0.31332
              19  58.785 0.08995  0.12431    0.31707    0.33248    0.23839    0.27523    0.35459    0.26798
              18  59.315 0.10658  0.14470    0.32004    0.32994    0.25280    0.28689    0.32058    0.23847
              17  59.698 0.12187  0.16335    0.31813    0.32398    0.26155    0.29318    0.29845    0.21949
              16  59.980 0.13586  0.18040    0.31366    0.31658    0.26626    0.29576    0.28421    0.20727
              15  60.194 0.14865  0.19597    0.30811    0.30886    0.26820    0.29586    0.27505    0.19931
              14  60.362 0.16033  0.21018    0.30232    0.30144    0.26828    0.29436    0.26908    0.19402
              13  60.498 0.17099  0.22315    0.29676    0.29462    0.26715    0.29184    0.26511    0.19038
              12  60.611 0.18071  0.23496    0.29164    0.28851    0.26526    0.28873    0.26238    0.18780
              11  60.707 0.18957  0.24569    0.28706    0.28311    0.26293    0.28532    0.26044    0.18588
              10  60.789 0.19762  0.25542    0.28301    0.27839    0.26037    0.28179    0.25901    0.18440
FEED                                0.25000               0.25000               0.25000               0.25000
              10  60.761 0.19625  0.25389    0.28324    0.27887    0.25989    0.28153    0.26062    0.16571
               9  61.182 0.20572  0.26245    0.29426    0.28589    0.27330    0.29210    0.22673    0.15956
               8  61.597 0.21642  0.27234    0.30303    0.29058    0.28650    0.30218    0.19405    0.13490
               7  62.006 0.22877  0.28405    0.30889    0.29242    0.29911    0.31141    0.16322    0.11212
               6  62.407 0.24341  0.29826    0.31120    0.29093    0.31064    0.31933    0.13475    0.09148
               5  62.804 0.26118  0.31589    0.30933    0.28560    0.32055    0.32540    0.10894    0.07311
               4  63.206 0.28321  0.33808    0.30268    0.27599    0.32813    0.32891    0.08598    0.05703
               3  63.620 0.31095  0.36621    0.29066    0.26163    0.33251    0.32898    0.06588    0.04317



               2  64.060 0.34611  0.40185    0.27271    0.24215    0.33261    0.32458    0.04856    0.03142
               1  64.538 0.39066  0.44660    0.24837    0.21731    0.32710    0.31448    0.03387    0.02161
  BOTTOMS                           0.44660               0.21731               0.31448               0.02161
```

I. PROBLEM IDENTIFICATION

CACHE COMPUTER PROGRAM

Name: David M. Watt, Jr.

Type: Self-standing

1. Title: Multicomponent Distillation--Design Case
2. Authors: Jean P. Leinroth, Jr. and David M. Watt, Jr. (at Cornell University during the development of the problem)
3. Organization name, address and telephone number: Procter & Gamble Co., Miami Valley Laboratories, P. O. Box 39175, Cincinnati, Ohio 45239, 513-738-1111.
4. Abstract:

For a multicomponent bubble point feed of known composition, this program calculates down tray-by-tray from the total condenser with specified distillate composition until the ratio of the mole fractions of the light and heavy keys is less than the corresponding ratio in the feed. This gives the number of trays above the feed. Similar tray-by-tray calculations from the reboiler with specified bottoms composition up the column until the ratio of the mole fractions of the light and heavy keys is greater than the corresponding ratio in the feed gives the number of trays below the feed. This calculation gives the total number of required trays for the separation, but it leaves a composition discontinuity at the feed tray. This design number of required trays can then be used in a column rating calculation to determine the actual distillate and bottoms compositions. (See CACHE problem "Multicomponent Distillation-Rating Case.)

Antoine constants are calculated from vapor pressure data, and Raoult's law is used to calculate vapor-liquid equilibrium constants. Constant molal overflow is assumed. Dew point and bubble point subroutines use the Newton-Raphson method and were developed for CACHE problem "Bubble and Dew Point Calculations with Ideal Mixtures."

5. Program Development:

5.1 Computer used: IBM 360 Model 44 5.2 Minimum core: 41 K

5.3 Operating environment: Batch 5.4 Language: Fortran IV

5.5 Typical run time: 1 min.20 sec. total 5.6 No. of Source Cards: 169

II. TECHNICAL DESCRIPTION

1. Problem Statement: The problem is to find the number of ideal stages to effect a specified multicomponent separation. For this example the following stream is fed as a liquid at its boiling point to the optimum point in the column:

	Moles per hour
n-Pentane	15
Hexane	35
Heptane	40
Octane	10

A distillate containing not over 0.01 mole fraction heptane is to be produced; the bottoms are to contain not over 0.005 mole fraction hexane. The column is to operate at atmospheric pressure. A total condenser is to be used. The reflux ratio is to be 1.8/1.

2. Problem Formulation and Technical Analysis: The components are numbered from lightest to heaviest. The light key is component 2 and the heavy key is component 3. For this design calculation it is reasonable to assume that the distillate contains nothing heavier than the heavy key (XD(4)=0) and that the bottoms contain nothing lighter than the light key (XB(1)=0). Hand calculations give the flow rates and compositions of both the distillate and the bottoms; these are inputs to the computer calculation.

On the computer the first step is to develop subroutines for calculating dew points and bubble points for the tray-to-tray calculations. Subroutines DEW and BUBBLE were commonly developed in an earlier homework assignment along with the input of required data and form the basis for CACHE problem "Bubble and Dew Point Calculations with Ideal Mixtures." For this mixture Raoult's law can be assumed, and only a vapor pressure correlation is necessary to determine vapor-liquid equilibria. For each component two vapor pressures are read in with the corresponding temperatures and two Antoine constants are calculated.

ALOG (PSTAR) = A + B/TK (1)

The CACHE problem "Bubble and Dew Point Calculations with Ideal Mixtures" shows the details of the Newton-Raphson solutions for both subroutines. Note that the final compositions are normalized to sum exactly to unity. The output of these subroutines is the temperature and equilibrium composition and is transmitted by COMMON block POT

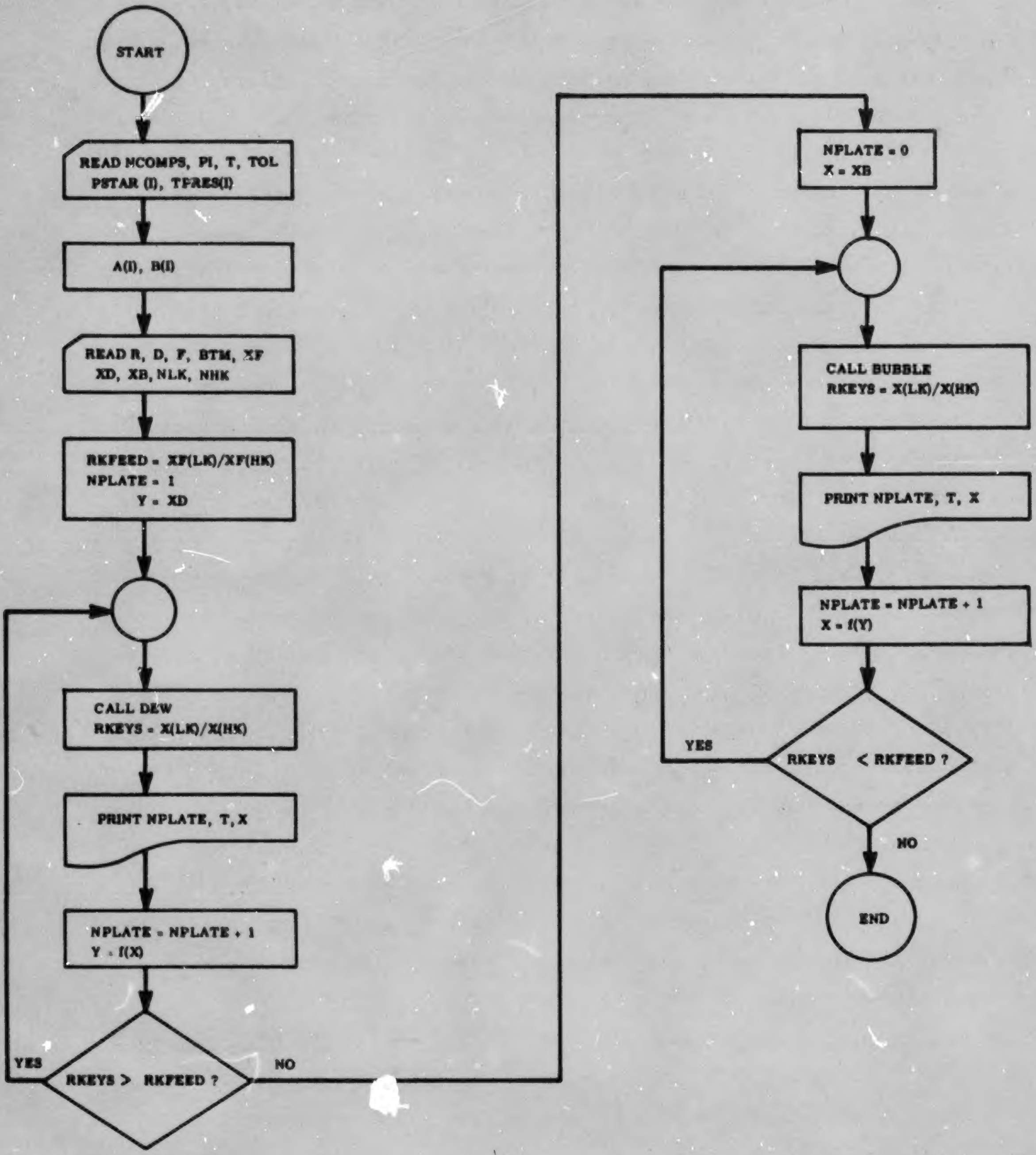
A combination of mass balances assuming constant molal overflow and equilibrium calculations using these subroutines enables tray-by-tray calculations down the column from the top tray, which has the same composition as the distillate since a total condenser is specified. Calculations are continued down the column until the ratio of the mole fractions of the light and heavy keys is less than the corresponding ratio in the feed. The number of trays stepped off in this fashion is a good approximation to the number of trays above the feed when liquid feed at its boiling point is used. Similar tray-by-tray calculations up the column starting from the reboiler with the same composition as the bottoms stream are continued until the ratio of the mole fractions of the light and heavy keys is greater than the corresponding ratio in the feed. This gives the number of trays below the feed.

This calculation gives the number of ideal stages required for this separation, but the calculations down the column to the feed tray do not give the same feed tray composition as is found by calculating up the column. This design number of trays can be used in a column rating calculation to determine the actual distillate and bottoms compositions.

3. Method of Solution: Step through the flow chart given in Fig. 1. First to be read in is the number of components, the total pressure, a reasonable guess of the temperature of the top plate, and the tolerance for the dew point and bubble point calculations. Vapor pressure data are then read in and Antoine constants are calculated for each component.

The column conditions are read in: the reflux ratio, the flow rates of the distillate, feed, and bottoms, and the composition vectors of the distillate, feed, and bottoms. With the input of the light and heavy key component numbers, the ratio of the mole fractions of the light and heavy keys in the feed stream is calculated. Several sums and products are put in memory to reduce the repetition of these calculations in each material balance.

Fig. 1. DESIGN CASE


START
READ NCOMPS, PI, T, TOL
PSTAR (I), TPRES(I)
A(I), B(I)
READ R, D, F, BTM, XF
XD, XB, NLK, NHK
RKFEED = XF(LK)/XF(HK)
NPLATE = 1
Y = XD
CALL DEW
RKEYS = X(LK)/X(HK)
PRINT NPLATE, T, X
NPLATE = NPLATE + 1
Y = f(X)
YES
RKEYS > RKFEED ?
NO
NPLATE = 0
X = XB
CALL BUBBLE
RKEYS = X(LK)/X(HK)
PRINT NPLATE, T, X
NPLATE = NPLATE + 1
X = f(Y)
YES
RKEYS < RKFEED ?
NO
END

The vapor composition on the top tray is initialized with the specified distillate composition to prepare for the repetitive tray-by-tray calculation down the column. A dew point calculation gives the temperature of the top tray and the liquid composition. Subroutine DEW is described in CACHE problem "Bubble and Dew Point Calculations with Ideal Mixtures." The ratio of the mole fractions of the light and heavy keys is calculated and the plate number, temperature, and liquid composition are printed out. The vapor composition on the next tray is found by a mass balance around the top of the column with the assumption of constant molal overflow. The ratio of the key components on this tray is then compared to this ratio in the feed; if it is larger, then the sequence of dew point calculation and mass balance is repeated; when it is smaller, the number of trays in the rectifying section has been found.

Finding the number of trays in the stripping section begins with initialization by setting the liquid composition vector equal to the bottoms and reboiler composition. A bubble point calculation gives the composition of the vapor rising to the first tray above the reboiler. The ratio of the mole fractions of the light and heavy keys is then calculated, and the plate number, temperature, and liquid composition are printed. The number zero is given for the reboiler. Using the vapor composition, a mass balance around the bottom of the column gives the liquid composition on the next tray up the column. If the ratio of the key components is less than the corresponding ratio in the feed, then this sequence of bubble point calculation and material balance is repeated for the next tray. When this ratio is greater than the key ratio in the feed, then the number of trays below the feed has been found, and the design is complete.

4. Range of Application: This is an extension of the McCabe-Thiele binary distillation method to multicomponent problems. Raoult's law is used; therefore, the mixtures must be ideal. This restriction could be removed by modifying the dew point and bubble point subroutines.

5. Output: All the input data are printed out with labels (Fig. 2). For each plate the temperature, composition, and number of iterations in the dew point or bubble point subroutine are printed out.

```
DESIGN CASE**SEPARATION OF PENTANE, HEXANE, HEPTANE, AND OCTANE


  4. COMPONENTS,      TOTAL PRESSURE=  760. MM HG
   ESTIMATE OF TOP TRAY TEMPERATURE IS      50. DEGREES C
   TOLERANCE CN DEW AND BUBBLE POINT CONVERGENCE IS     0.00100


 VAPOR PRESSURE DATA AND ANTOINE CONSTANTS BY COMPONENT

I=1        P*=     760.00      AT T=      36.10
           P*=    3800.00      AT T=      92.40
           A=      17.0789100         B=  -3228.7360000

I=2        P*=     760.00      AT T=      68.70
           P*=    3800.00      AT T=     131.70
           A=      16.9720300         B=  -3532.7410000

I=3        P*=     760.00      AT T=      98.40
           P*=    3800.00      AT T=     165.70
           A=      17.1245400         B=  -3896.4420000

I=4        P*=     760.00      AT T=     125.50
           P*=    3800.00      AT T=     196.20
           A=      17.3143300         B=  -4256.3860000


REFLUX RATIO=      1.800          FEED=   100.000          DISTILLATE=     50.250

                                                             BOTTOMS=     49.750
             XF                    XD                    XB
         0.14999990           0.29799990           0.00000000
         0.35000000           0.69199990           0.00500000
         0.39999990           0.01000000           0.79500000
         0.10000000           0.00000000           0.19999990

LIGHT KEY= 2           HEAVY KEY= 3
```

```
STEP DOWN COLUMN TO FEED TRAY


PLATE NO=     1           T=  62.481           ITERATIONS=    4.
                   COMPONENT= 1         X= 0.13106          Y= 0.29800
                   COMPONENT= 2         X= 0.83819          Y= 0.69200
                   COMPONENT= 3         X= 0.03075          Y= 0.01000
                   COMPONENT= 4         X= 0.00000          Y= 0.00000

PLATE NO=     2           T=  65.769           ITERATIONS=    3.
                   COMPONENT= 1         X= 0.07638          Y= 0.19068
                   COMPONENT= 2         X= 0.85951          Y= 0.78598
                   COMPONENT= 3         X= 0.06411          Y= 0.02334
                   COMPONENT= 4         X= 0.00000          Y= 0.00000

PLATE NO=     3           T=  67.655           ITERATIONS=    3.
                   COMPONENT= 1         X= 0.05910          Y= 0.15553
                   COMPONENT= 2         X= 0.82546          Y= 0.79968




                   COMPONENT= 3         X= 0.11544          Y= 0.04479
                   COMPONENT= 4         X= 0.00000          Y= 0.00000

PLATE NO=     4           T=  69.497           ITERATIONS=    3.
                   COMPONENT= 1         X= 0.05215          Y= 0.14442
                   COMPONENT= 2         X= 0.75931          Y= 0.77779
                   COMPONENT= 3         X= 0.18853          Y= 0.07778
                   COMPONENT= 4         X= 0.00000          Y= 0.00000
```

```
PLATE NO=     5           T=  71.726          ITERATIONS=   3.
                    COMPONENT= 1        X= 0.04755          Y= 0.13996
                    COMPONENT= 2        X= 0.67148          Y= 0.73527
                    COMPONENT= 3        X= 0.28097          Y= 0.12477
                    COMPONENT= 4        X= 0.00000          Y= 0.00000

PLATE NO=     6           T=  74.282          ITERATIONS=   3.
                    COMPONENT= 1        X= 0.04345          Y= 0.13700
                    COMPONENT= 2        X= 0.57488          Y= 0.67881
                    COMPONENT= 3        X= 0.38168          Y= 0.18420
                    COMPONENT= 4        X= 0.00000          Y= 0.00000

PLATE NO=     7           T=  76.835          ITERATIONS=   3.
                    COMPONENT= 1        X= 0.03981          Y= 0.13436
                    COMPONENT= 2        X= 0.48491          Y= 0.61671
                    COMPONENY= 3        X= 0.47528          Y= 0.24894
                    COMPONENT= 4        X= 0.00000          Y= 0.00000

PLATE NO=     8           T=  79.034          ITERATIONS=   3.
                    COMPONENT= 1        X= 0.03693          Y= 0.13202
                    COMPONENT= 2        X= 0.41258          Y= 0.55887
                    COMPONENT= 3        X= 0.55049          Y= 0.30911
                    COMPONENT= 4        X= 0.00000          Y= 0.00000
THE FEED SHOULD BE INTRODUCED BELOW TRAY    8 FROM THE TOP OF THE COLUMN.
```

```
STEP UP FROM THE REBOILER


PLATE  NO=     0            T= 102.215               ITERATIONS=    4.
                     COMPONENT= 1           X= 0.00000           Y= 0.00000
                     COMPONENT= 2           X= 0.00500           Y= 0.01259
                     COMPONENT= 3           X= 0.79500           Y= 0.88435
                     COMPONENT= 4           X= 0.20000           Y= 0.10306

PLATE  NO=     1            T= 100.474               ITERATIONS=    2.
                     COMPONENT= 1           X= 0.00000           Y= 0.00000
                     COMPONENT= 2           X= 0.01061           Y= 0.02553
                     COMPONENT= 3           X= 0.86101           Y= 0.91177
                     COMPONENT= 4           X= 0.12838           Y= 0.06270

PLATE  NO=     2            T=  99.400               ITERATIONS=    2.
                     COMPONENT= 1           X= 0.00000           Y= 0.00000

                     COMPONENT= 2           X= 0.02017           Y= 0.04728
                     COMPONENT= 3           X= 0.88127           Y= 0.90611
                     COMPONENT= 4           X= 0.09856           Y= 0.04661

PLATE  NO=     3            T=  98.422               ITERATIONS=    2.
                     COMPONENT= 1           X= 0.00000           Y= 0.00000
                     COMPONENT= 2           X= 0.03624           Y= 0.08286
                     COMPONENT= 3           X= 0.87709           Y= 0.87737
                     COMPONENT= 4           X= 0.08668           Y= 0.03977

PLATE  NO=     4            T=  97.152               ITERATIONS=    2.
                     COMPONENT= 1           X= 0.00000           Y= 0.00000
                     COMPONENT= 2           X= 0.06252           Y= 0.13833
                     COMPONENT= 3           X= 0.85585           Y= 0.82567
                     COMPONENT= 4           X= 0.08163           Y= 0.03600
```

```
PLATE NO=      5            T=   95.308            ITERATIONS=     3.
                     COMPONENT= 1          X= 0.00000               Y= 0.00000
                     COMPONENT= 2          X= 0.10350               Y= 0.21843
                     COMPONENT= 3          X= 0.81766               Y= 0.74872
                     COMPONENT= 4          X= 0.07884               Y= 0.03285

PLATE NO=      6            T=   92.841            ITERATIONS=     3.
                     COMPONENT= 1          X= 0.00000               Y= 0.00000
                     COMPONENT= 2          X= 0.16268               Y= 0.32182
                     COMPONENT= 3          X= 0.76081               Y= 0.64870
                     COMPONENT= 4          X= 0.07651               Y= 0.02949

PLATE NO=      7            T=   89.881            ITERATIONS=     3.
                     COMPONENT= 1          X= 0.00000               Y= 0.00000
                     COMPONENT= 2          X= 0.23906               Y= 0.43710
                     COMPONENT= 3          X= 0.68692               Y= 0.53696
                     COMPONENT= 4          X= 0.07403               Y= 0.02595
```

```
PLATE NO=     8          T=  86.836          ITERATIONS=    3.
                    COMPONENT= 1        X= 0.00000            Y= 0.00000
                    COMPONENT= 2        X= 0.32422            Y= 0.54594
                    COMPONENT= 3        X= 0.60436            Y= 0.43140
                    COMPONENT= 4        X= 0.07141            Y= 0.02267

PLATE NO=     9          T=  84.177          ITERATIONS=    3.
                    COMPONENT= 1        X= 0.00000            Y= 0.00000
                    COMPONENT= 2        X= 0.40463            Y= 0.63332
                    COMPONENT= 3        X= 0.52638            Y= 0.34663
                    COMPONENT= 4        X= 0.06899            Y= 0.02005

PLATE NO=    10          T=  82.177          ITERATIONS=    3.
                    COMPONENT= 1        X= 0.00000            Y= 0.00000
                    COMPONENT= 2        X= 0.46919            Y= 0.69458
                    COMPONENT= 3        X= 0.46376            Y= 0.28720
                    COMPONENT= 4        X= 0.06706            Y= 0.01822
THERE ARE    10 PLATES PLUS THE REBOILER IN THE STRIPPING SECTION.
```

6. References and Data: This method of using the ratio of the light and heavy keys to determine the number of required trays is discussed by C. S. Robinson and E. R. Gilliland, "Elements of Fractional Distillation," 4th Ed., p. 245, McGraw-Hill, New York, 1950. There are many sources of vapor pressure data, including J. H. Perry's Chemical Engineering Handbook.

III. EDUCATIONAL ASPECTS

1. Description of past usage: This is described in more detail in an article accepted for publication by Chemical Engineering Education, "Building a Multicomponent Distillation Computer Program" by Jean P. Leinroth, Jr. and David M. Watt, Jr. This problem was used for several years in the junior year chemical engineering course on stage processes at Cornell University. The multicomponent distillation program was developed in three assignments: (1) writing dew point and bubble point routines, (2) determining the approximate number of plates required in the column by a non-iterative scheme based on assumed overhead and bottoms compositions, and (3) rating the column to determine the actual performance and distribution of components by an iterative technique. This problem is step (2) and descriptions of steps (1) and (3) are also in CACHE. Two weeks were allowed for each assignment to permit adequate time for debugging. After the initial writing of each program was completed, the debugging load was sufficiently light that additional problems not requiring computer solution could be assigned in the interim.

2. Concepts and Techniques Taught: The students taking the course had received an introduction to digital computers in a freshman course; consequently, the lectures on computing in this course emphasized flow charts and the assembly of large, complex computer programs from relatively simple subprograms. Since the problem is an extension of the McCabe-Thiele method to multicomponent systems, the flow chart analysis and computer algorithm enable the student to visualize each step in the McCabe-Thiele method, thus helping to overcome the usual tendency for a student to use the McCabe-Thiele method without knowing what each step represents. Quiz questions relate the flow chart for this problem to other stage processes such as liquid-liquid extraction, and the concept of an equilibrium stage is made very clear.

3. Student Response: During the several years in which this problem sequence has been used, the problem generated enthusiasm which carried over into other elements of the course. In addition, learning to use flow charts while developing the computer algorithms enabled students to use with confidence existing library subprograms, not only for other parts of this course, but in other courses as well.

IV. PROGRAM DESCRIPTION

1. External Description:
   a. Input data format (the comment cards and the following list give a description of each variable):

Card Set 1:	Columns 2-80, PNAME, the program name, A Format.
Card Set 2:	ANCOMP,PI,T,TOL: Format 4F20.5. ANCOMP, the number of components, must be less than or equal to 10.
Card Set 3:	one card per component, PSTAR(1), TPRES(1), PSTAR(2), TPRES(2); Format 4F20.5
Card Set 4:	R,F,D,BTM; Format 4F20.5
Card Set 5:	one card per component(I), XF(I),XD(I),XB(I); Format 3F20.5
Card Set 6:	NLK,NHK; Format 2I20

   b. Output Data: these are all labeled.
   c. IN and IO, the input and output files or units are read in as DATA.

2. Program Variables: Variable specification, either fixed or floating point, follows standard FORTRAN. The listing for subroutines BUBBLE and DEW is found with CACHE problem "Bubble and Dew Point Calculations with Ideal Mixtures."

A(I), I .LE. 10, first Antoine constant, component I, for vapor pressures in mm.Hg

AITER, iteration count used in subroutines DEW and BUBBLE

ANCOMP=NCOMP, .LE. 10, the number of components

B(I), second Antoine constant for component I, ^{o}K

BL, liquid flow rate down the column below the feed, moles/hr.

BOBL=BTM/BL

BTM, bottoms flow rate, moles/hr.

D, distillate flow rate, moles/hr.

DOV = D/V

F, feed flow rate, moles/hr.

NCOMPS, number of components, .LE. 10

NHK, the component number of the heavy key

NLK, the component number of the light key

PI, total pressure, mm.Hg

PNAME, the problem name, A Format

PSTAR(J), vapor pressure input datum, mm.Hg, corresponding to TPRES(J)

R, reflux ratio

RD, liquid flow rate down the column above the feed, moles/hr.

RDOV = RD/V

RKEYS, the ratio of the mole fractions of the light and heavy key components in the column

RKFEED, the ratio of the mole fractions of the light and heavy key components in the feed

T, temperature, $^{\circ}$C

TK, temperature, $^{\circ}$K

TOL, tolerance for convergence in subroutines DEW and BUBBLE

TPRES(J), input temperature, $^{\circ}$C, corresponding to PSTAR(J)

V, vapor flow rate in the column above the feed, moles/hr.

VB, vapor flow rate in the column below the feed, moles/hr.

VBOBL = VB/BL

X(I), liquid mole fraction, component I

XB(I), bottoms liquid mole fraction, component I

XD(I), distillate liquid mole fraction, component I

XF(I), feed liquid mole fraction, component I

Y(I), vapor mole fraction, component I

3. Program Logic: This is discussed in Section II (3) along with the flow chart, Fig. 1.

V. - CARD LISTING

See the following pages.

```
    $JOB             320505075,KP=29,TIME=60
    C                                                                       MAIN    1
    C     MULTICCMPONENT CISTILLATION CALCULATION OF REQUIRED TRAYS         MAIN    2
    C     BUBBLE POINT FEED ANC REFLUX,  TOTAL CONDENSER,  REBOILER         MAIN    3
    C     NCCMPS=NUMBER OF COMPONENTS,  FLOW RATES IN MOLES/HOUR            MAIN    4
    C     F=FEEC,  D= DISTILLATE,  BTM= BOTTOMS FLOW RATES. . R=REFLUX RATIO MAIN   5
    C     RD=R*D= LIQUID FLOW ABOVE FEED, BL= LIQUID FLOW RATE BELCW FEED   MAIN    6
    C     V,VB= VAPOR FLOW RATES ABOVE AND BELOW FEED                       MAIN    7
    C     Y(I),X(I)=VAPOR, LIQUID MOLE FRACTIONS. YOX=Y/X=EQUILIBRIUM K VALUEMAIN   8
    C     NLK,NHK= LIGHT AND HEAVY KEYS..T=DEGREES C, TK= DEGREES K         MAIN    9
    C     PI=TOTAL PRESSURE,TORR.  PSTAR=VAPOR PRESSURE, TORR               MAIN   10
    C     A,B=ANTCINE CONSTANTS....  LN(PSTAR)=A+B/TK                       MAIN   11
 1         CCMMCN /POT/ X,Y,A,B,T,TK,PI,AITER,NCOMPS,TOL                    MAIN   12
 2         DIMENSION X(10),Y(10),A(10),B(10),TPRES(2),PSTAR(2)              MAIN   13
 3         DIMENSION XF(10),XD(10),XB(10)                                   MAIN   14
 4         DIMENSION PNAME(20)                                              MAIN   15
 5         DATA IN,IO/5,6/
    C     PNAME IS THE PROBLEM NAME WRITTEN ON ONE CARD EXCEPT FOR COLUMN ONEMAIN  17
 6       5 READ (IN,109) PNAME                                              MAIN   18
 7         WRITE (IO,110) PNAME                                             MAIN   19
 8     109 FCRMAT (20A4)                                                    MAIN   20
 9     110 FORMAT (1H1,20A4)                                                MAIN   21
    C     READ IN NUMBER OF COMPONENTS,CONSTANT TOTAL PRESSURE,GUESS OF TEMP MAIN  22
    C     OF TOP PLATE, TOLERANCE FOR CONVERGENCE OF DEW AND BUBBLE         MAIN   23
10         READ (IN,100) ANCOMP, PI, T, TOL                                 MAIN   24
11     100 FCRMAT (4F20.8)                                                  MAIN   25
```

```
      WRITE (IO,107) ANCOMP,PI,T,TOL                                    MAIN  26
  107 FORMAT (//,1X,F5.0,12H COMPONENTS,,5X,15HTOTAL PRESSURE=,F6.0,    MAIN  27
     16H MM HG ,/,5X,38HESTIMATE OF TOP TRAY TEMPERATURE IS   ,F5.0,    MAIN  28
     210H DEGREES C ,/,5X, 49HTOLERANCE ON DEW AND BUBBLE POINT CONVERGEMAIN  29
     3NCE IS      ,F10.5)                                               MAIN  30
      NCOMPS=ANCOMP                                                     MAIN  31
      IF (NCOMPS .LE.0)STOP                                             MAIN  32
      TK=T+273.                                                         MAIN  33
C       FOR EACH COMPONENT READ IN TWO VAPOR PRESSURES AND TEMPERATURES MAIN  34
C       AND COMPUTE THE ANTOINE CONSTANTS                               MAIN  35
      WRITE (IO,102)                                                    MAIN  36
  102 FORMAT (//,70H  VAPOR PRESSURE DATA AND ANTOINE CONSTANTS BY COMPOMAIN  37
     1NENT                             )                                MAIN  38
      DO 90 I=1,NCOMPS                                                  MAIN  39
      READ (IN,100) PSTAR(1),TPRES(1),PSTAR(2),TPRES(2)                 MAIN  40
      B(I)=(ALOG(PSTAR(2))-ALOG(PSTAR(1)))/(1.0/(TPRES(2)+273.0)        MAIN  41
     1-1.0/(TPRES(1)+273.0))                                            MAIN  42
      A(I)=ALOG(PSTAR(1))-B(I)/(TPRES(1)+273.0)                         MAIN  43
   90 WRITE (IO,101) I,PSTAR(1),TPRES(1),PSTAR(2),TPRES(2),A(I),B(I)    MAIN  44
  101 FORMAT (/,3H I=,I1,6X,3HP*=,F10.2,5X,5HAT T=,F10.2,/,10X,3HP*=,   MAIN  45
     1 F10.2,5X,5HAT T=,F10.2,/,10X,2HA=,F15.7,8X,2HB=,F15.7)           MAIN  46
C                                                                       MAIN  47
C     READ IN COLUMN LIQUID FLOW RATES AND REFLUX RATIO                 MAIN  48
      READ (IN,100) R,F,D,BTM                                           MAIN  49
      WRITE (IO,103) R,F,D,BTM                                          MAIN  50
  103 FORMAT (//,14H REFLUX RATIO=,F10.3,10X,5HFEED=,F10.3,10X,         MAIN  51
     111HDISTILLATE=,F10.3,10X,8HBOTTOMS=,F10.3)                        MAIN  52
      WRITE (IO,104)                                                    MAIN  53
  104 FORMAT (//,15X,2HXF,20X,2HXD,20X,2HXB)                            MAIN  54
C    READ IN COMPOSITIONS OF FEED, DISTILLATE, BOTTOMS                  MAIN  55
      DO 150 I=1,NCOMPS                                                 MAIN  56
      READ (IN,100) XF(I),XD(I),XB(I)                                   MAIN  57
  150 WRITE (IO,100) XF(I),XD(I),XB(I)                                  MAIN  58
C     READ IN THE COMPONENT NUMBER OF THE LIGHT AND HEAVY KEYS          MAIN  59
```

```
      READ (IN,105) NLK,NHK                                             MAIN  60
  105 FORMAT (4I20)                                                     MAIN  61
      WRITE (IO,106) NLK,NHK                                            MAIN  62
  106 FORMAT (/,11H LIGHT KEY=,I2,10X,10HHEAVY KEY=,I2,//)              MAIN  63
C     STARTING CALCULATIONS AT TOP AND INITIALIZATION                   MAIN  64
      RD=R*D                                                            MAIN  65
      V=D+RD                                                            MAIN  66
      RDOV=RD/V                                                         MAIN  67
      DOV=D/V                                                           MAIN  68
      NPLATE=1                                                          MAIN  69
C     SET COMPOSITION OF TOP PLATE = DISTILLATE COMPOSITION             MAIN  70
      DO 160 I=1,NCOMPS                                                 MAIN  71
  160 Y(I)=XD(I)                                                        MAIN  72
C   THE RATIO OF THE MOLE FRACTIONS OF LIGHT AND HEAVY KEYS IS USED TO  MAIN  73
C     INDICATE THE LOCATION OF THE FEED TRAY. PLATES ARE STEPPED OFF FROMMAIN  74
C     THE TOP AS LONG AS THIS KEY RATIO, RKEYS, IS GREATER THAN THE KEY  MAIN  75
C     RATIO IN THE FEED, RKFEED.  THEN PLATES ARE STEPPED OFF UP FROM    MAIN  76
C     THE REBOILER AS LONG AS RKEYS IS LESS THAN RKFEED.                MAIN  77
      RKFEED=XF(NLK)/XF(NHK)                                            MAIN  78
      WRITE (IO,170)                                                    MAIN  79
  170 FORMAT (30H STEP DOWN COLUMN TO FEED TRAY  ,/)                    MAIN  80
  175 CALL DEW                                                          MAIN  81
      RKEYS=X(NLK)/X(NHK)                                               MAIN  82
      WRITE (IO,180) NPLATE,T,AITER                                     MAIN  83
  180 FORMAT (//,10H PLATE NO=,I5,10X,2HT=,F8.3,10X,11HITERATIONS=,F5.0)MAIN  84
      DO 190 I=1,NCOMPS                                                 MAIN  85
  190 WRITE (IO,200) I,X(I),Y(I)                                        MAIN  86
  200 FORMAT (20X,11H COMPONENT=,I2,7X,2HX=,F8.5,10X,2HY=,F8.5)         MAIN  87
      NPLATE=NPLATE+1                                                   MAIN  88
      DO 210 I=1,NCOMPS                                                 MAIN  89
  210 Y(I)=RDOV*X(I)+DOV*XD(I)                                          MAIN  90
      IF (RKEYS .GT.RKFEED) GO TO 175                                   MAIN  91
      NPLATE=NPLATE-1                                                   MAIN  92
      WRITE (IO,220) NPLATE                                             MAIN  93
  220 FORMAT (42H THE FEED SHOULD BE INTRODUCED BELOW TRAY   ,I4,       MAIN  94
     128H FROM THE TOP OF THE COLUMN.    )                              MAIN  95
C     INITIALIZE FOR STRIPPING SECTION                                  MAIN  96
      BL=RD+F                                                           MAIN  97
      VB=V                                                              MAIN  98
      VBOBL=VB/BL                                                       MAIN  99
      BOBL=BTM/BL                                                       MAIN 100
      NPLATE=0                                                          MAIN 101
C     SET THE REBOILER COMPOSITION = THE BOTTOMS COMPOSITION.           MAIN 102
      DO 280 I=1,NCOMPS                                                 MAIN 103
  280 X(I)=XB(I)                                                        MAIN 104
      WRITE (IO,285)                                                    MAIN 105
  285 FORMAT (//,30H STEP UP FROM THE REBOILER       ,/)                MAIN 106
  290 CALL BUBBLE                                                       MAIN 107
      RKEYS=X(NLK)/X(NHK)                                               MAIN 108
      WRITE (IO,180) NPLATE,T,AITER                                     MAIN 109
      DO 300 I=1,NCOMPS                                                 MAIN 110
  300 WRITE (IO,200) I,X(I),Y(I)                                        MAIN 111
      NPLATE=NPLATE+1                                                   MAIN 112
      DO 310 I=1,NCOMPS                                                 MAIN 113
  310 X(I)=VBOBL*Y(I)+BOBL*XB(I)                                        MAIN 114
      IF(RKEYS .LT.RKFEED) GO TO 290                                    MAIN 115
      NPLATE=NPLATE-1                                                   MAIN 116
      WRITE (IO,320) NPLATE                                             MAIN 117
  320 FORMAT (11H THERE ARE  ,I4,55H PLATES PLUS THE REBOILER IN THE STRMAIN 118
     1IPPING SECTION.          )                                        MAIN 119


       GO TO 5
      END                                                               MAIN 121
      SUBROUTINE DEW                                                    DEW    1
C     DEW COMPUTES THE DEW POINT TEMPERATURE AND EQUILIBRIUM LIQUID     DEW    2
C     COMPOSITION FOR A GIVEN VAPOR COMPOSITION                         DEW    3
C     THE NEWTON-RAPHSON METHOD IS USED FOR CONVERGENCE TO TOLERANCE TOL DEW   4
      COMMON /POT/ X,Y,A,B,T,TK,PI,AITER,NCOMPS,TOL                     DEW    5
      DIMENSION X(10),Y(10),A(10),B(10)                                 DEW    6
      AITER=1.                                                          DEW    7
    1 FOFT=1.                                                           DEW    8
      DFOFT=0.                                                          DEW    9
      DO 2 I=1,NCOMPS                                                   DEW   10
      YOX=(EXP(A(I)+B(I)/TK))/PI                                        DEW   11
      X(I)=Y(I)/YOX                                                     DEW   12
      FOFT=FOFT-X(I)                                                    DEW   13
    2 DFOFT=DFOFT-X(I)*B(I)/(TK**2)                                     DEW   14
      IF(ABS(FOFT) .LT. TOL) GO TO 3                                    DEW   15
      TK=TK-FOFT/DFOFT                                                  DEW   16
      AITER=AITER+1.                                                    DEW   17
      IF (AITER .LT. 15) GO TO 1                                        DEW   18
    3 SUMX=1.0-FOFT                                                     DEW   19
      DO 4 I=1,NCOMPS                                                   DEW   20
    4 X(I)=X(I)/SUMX                                                    DEW   21
      T=TK-273.                                                         DEW   22
      RETURN                                                            DEW   23
      END                                                               DEW   24
      SUBROUTINE BUBBLE                                                 BUBL   1
C     BUBBLE COMPUTES THE BUBBLE POINT TEMPERATURE AND VAPOR COMPOSITION BUBL   2
C     IN EQUILIBRIUM WITH A GIVEN LIQUID COMPOSITION                    BUBL   3
C     THE NEWTON-RAPHSON METHOD IS USED FOR CONVERGENCE TO TOLERANCE TOL BUBL   4
      COMMON /POT/ X,Y,A,B,T,TK,PI,AITER,NCOMPS,TOL                     BUBL   5
      DIMENSION X(10),Y(10),A(10),B(10)                                 BUBL   6
      AITER=1.                                                          BUBL   7
   10 FOFT=1.                                                           BUBL   8
      DFOFT=0.                                                          BUBL   9
      DO 20 I=1,NCOMPS                                                  BUBL  10
      YOX=(EXP(A(I)+B(I)/TK))/PI                                        BUBL  11
      Y(I)=YOX*X(I)                                                     BUBL  12
      FOFT=FOFT-Y(I)                                                    BUBL  13
   20 DFOFT=DFOFT+Y(I)*B(I)/(TK**2)                                     BUBL  14
      IF (ABS(FOFT).LT.TOL)GO TO 30                                     BUBL  15
      TK=TK-FOFT/DFOFT                                                  BUBL  16
      AITER=AITER+1.                                                    BUBL  17
      IF (AITER .LT. 15) GO TO 10                                       BUBL  18
   30  SUMY=1.0-FOFT                                                    BUBL  19
      DO 40 I=1,NCOMPS                                                  BUBL  20
   40 Y(I)=Y(I)/SUMY                                                    BUBL  21
      T=TK-273.                                                         BUBL  22
      RETURN                                                            BUBL  23
      END                                                               BUBL  24
```

I. PROBLEM IDENTIFICATION

CACHE COMPUTER PROGRAM

Name: David M. Watt, Jr.

Type: Self-standing

1. Title: Multicomponent Distillation--Rating Case
2. Authors: Jean P. Leinroth, Jr., and David M. Watt, Jr., (at Cornell University during the development of the problem)
3. Organization name, address and telephone number:
   Procter & Gamble, P. O. Box 39175, Cincinnati, Ohio 45239
   513-738-1111
4. Abstract:

For a multicomponent liquid feed to a specified distillation column, the exact distillate and bottoms compositions are calculated using the Thiele-Geddes iterative technique. Bubble point and dew point subroutines were developed for CACHE problem "Bubble and Dew Point Calculations with Ideal Mixtures" and are used with this program. The number of ideal stages required above and below the feed can be found with the CACHE program "Multicomponent Distillation--Design Case." This "Design Case" program is the basis for building the "Rating Case" program and enables the student to complete the problem in a single assignment.

In this iterative method calculations proceed from an estimate of the distillate composition down to the feed tray and from an estimate of the bottoms composition up to the feed tray. The ratio of these two calculated feed tray compositions is used to improve the estimates of the distillate and bottoms compositions. About ten iterations are usually sufficient for satisfactory convergence.

5. Program Development:

5.1 Computer used: IBM 360 Model 44 5.2 Minimum core: 43K

5.3 Operating environment: Batch 5.4 Language: Fortran IV

5.5 Typical run time: 1 min. 40 sec. total 5.6 No. of Source Cards: 226

II. TECHNICAL DESCRIPTION

1. Problem Statement: (The form of either "a" or "b" can be used.)

a. Having used the CACHE problem "Multicomponent Distillation--Design Case" to determine the number of ideal stages required above the feed tray and below the feed tray, find the exact distillate and bottoms composition for the example used in the "Design Case" problem.

b. A given column (the "Design Case") has a total condenser, 8 ideal plates above the feed, 10 ideal plates below the feed, and a reboiler. For the following feed to the column find the distillate and bottoms compositions using the Thiele-Geddes method. The column operates at 1 atm total pressure, and the reflux ratio is 1.8/1. The condenser is set to give a distillate flow rate of 50.25 moles/hr.

	Moles/hour
n-Pentane	15
Hexane	35
Heptane	40
Octane	10

2. Method of Solution: Only modifications to the CACHE problem "Multicomponent Distillation--Design Case" will be discussed here since in that problem all the necessary stage-to-stage calculations were developed. The only additional input data are NABOVE, the number of trays above the feed, and NBELOW, the number of trays below the feed. No estimates of distillate or bottoms compositions can be zero; therefore, for near zero compositions of the distillate or bottoms a mole fraction of 10^{-7} is used.

For calculational purposes the column is split into two parts: A, above the feed, and B, below the feed. AIN, the input to A must equal AOUT, the output from A, and similarly, BIN, the input to B, must equal BOUT, the output from B. These criteria are used to determine convergence.

Following the flow chart in Fig. 1, the data input and initial calculations are essentially the same as for the "Design Case" problem. With the initial estimate of the distillate composition, the calculations proceed down NABOVE plates to the feed tray and AOUT and BIN are computed by component. From the initial estimate of the bottoms composition, calculations proceed up the column for the reboiler and NBELOW plates, to the feed tray, and AIN and BOUT are computed by component. The following algorithm is used to reduce the mismatch between AIN and AOUT and between BIN and BOUT:

$$\left.\frac{XD(I)}{XB(I)}\right|_{new} = \Theta(I) * \left.\frac{XD(I)}{XB(I)}\right|_{old} \qquad (1)$$

where XD(I) = distillate mole fraction, component I

XB(I) = bottoms mole fraction, component I

$$\Theta(I) = \left[\frac{AIN(I)}{AOUT(I)} * \frac{BOUT(I)}{BIN\ (I)}\right]^{1/2} \qquad (2)$$

It will be noted that if $\Theta(I)$ is greater than unity, the next estimate of XD(I) will be increased and the next estimate of XB(I) will be decreased. The square root is used to evaluate $\Theta(I)$ rather than a linear relationship in order to reduce instability. Combining this new ratio of XD(I)/XB(I) with a mass balance gives the new distillate and bottoms compositions for the next iteration. Unfortunately, these mole fractions do not necessarily sum to one and a factor "C" is calculated to correct $\Theta(I)$ so that the distillate and bottoms mole fractions sum to one.

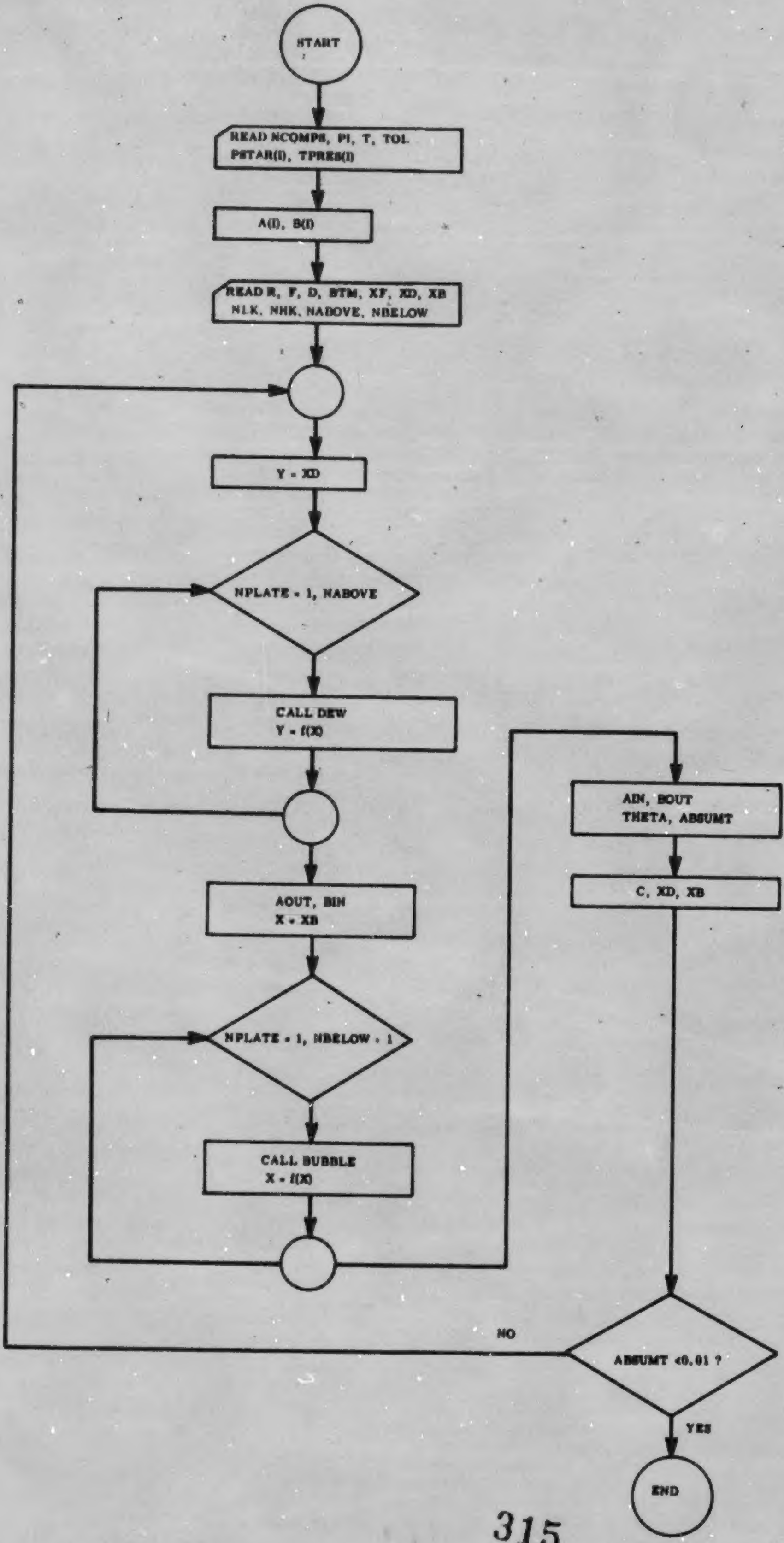
$$\left.\frac{XD(I)}{XB(I)}\right|_{new} = C * \Theta(I) * \left.\frac{XD(I)}{XB(I)}\right|_{old} \qquad (3)$$

"C" is calculated by a Newton-Raphson iteration using an initial estimate of C = 1.

At this point in the flow chart (Fig. 1), the new values of the distillate and bottoms compositions are known and it is necessary to decide whether another iteration is necessary. Since each $\Theta(I)$ approaches unity, ABSUMT converges arbitrarily close to zero and a tolerance of 0.01 to 0.03 is usually sufficient.

$$ABSUMT = \sum_{I=1}^{NCOMPS} \left| 1.0- \ THETA(I) \right| \qquad (4)$$

Fig. 1. RATING CASE


START
READ NCOMPS, PI, T, TOL
PSTAR(I), TPRES(I)
A(I), B(I)
READ R, F, D, BTM, XF, XD, XB
NLK, NHK, NABOVE, NBELOW
Y = XD
NPLATE = 1, NABOVE
CALL DEW
Y = f(X)
AOUT, BIN
X = XB
NPLATE = 1, NBELOW + 1
CALL BUBBLE
X = f(X)
AIN, BOUT
THETA, ABSUMT
C, XD, XB
NO
ABSUMT <0.01 ?
YES
END

If ABSUMT is greater than 0.01, the entire calculation through the column is repeated with the new distillate and bottoms compositions. When the iterations converge to ABSUMT less than 0.01, a final calculation through the column is made to print out the compositions and temperatures of each plate. Subroutine OUT prints out the plate composition and temperature.

3. Range of Application: In this extension of the McCabe-Thiele binary distillarion method to multicomponent systems, the distillate and bottoms compositions are iteratively improved until an integral number of ideal stages are used. All the assumptions used in the McCabe-Thiele method apply for this problem, particularly the constant molal overflow assumption. The Raoult's law assumption used for this problem could be removed by modifying the dew point and bubble point subroutines.

4. Output: All the input data are printed out with labels (Fig. 2). After each iteration ABSUMT, C, and vectors THETA, XD, and XB are printed out with labels. After convergence, all the plate compositions and temperatures are printed out with labels (Fig. 2).

5. References and Data: This application of the Thiele-Geddes method was presented by A. M. Peiser in Chemical Engineering 67, No. 14, 129 (1960). There are many sources of vapor pressure data, including J. H. Perry's Chemical Engineering Handbook.

III. EDUCATIONAL ASPECTS

These are described in the CACHE problem "Multicomponent Distillation--Design Case" and in an article accepted for publication by Chemical Engineering Education, "Building a Multicomponent Distillation Computer Program" by Jean P. Leinroth, Jr., and David M. Watt, Jr.

IV. PROGRAM DESCRIPTION

1. External Description:
   a. Input data format (the comment cards and the following list give a description of each variable):
      Card Set 1: Columns 2-80; PNAME, the program name, A Format.
      Card Set 2: ANCOMP, PI, T, TOL; Format 4F20.5.
      Card Set 3: one card per component, PSTAR(I), TPRES(1), PSTAR(2), TPRES(2)

```
RATING CASE FOR SEPARATION OF PENTANE, HEXANE, HEPTANE, AND OCTANE


   4. COMPONENTS,      TOTAL PRESSURE=  760. MM HG
    ESTIMATE OF TOP TRAY TEMPERATURE IS      50. DEGREES C
    TOLERANCE ON DEW AND BUBBLE POINT CONVERGENCE IS     0.00100


 VAPOR PRESSURE DATA AND ANTOINE CONSTANTS BY COMPONENT

I=1        P*=     760.00       AT T=      36.10
           P*=    3800.00       AT T=      92.40
           A=      17.0789100          B=  -3228.7360000

I=2        P*=     760.00       AT T=      68.70
           P*=    3800.00       AT T=     131.70
           A=      16.9720300          B=  -3532.7410000

I=3        P*=     760.00       AT T=      98.40
           P*=    3800.00       AT T=     165.70
           A=      17.1245400          B=  -3896.4420000

I=4        P*=     760.00       AT T=     125.50
           P*=    3800.00       AT T=     196.20
           A=      17.3143300          B=  -4256.3860000


REFLUX RATIO=      1.800          FEED=    100.000          DISTILLATE=     50.250
                                                              BOTTOMS=     49.750

               XF                       XD                       XB
           0.14999990               0.29799990               0.00000010
           0.35000000               0.69199990               0.00500000
           0.39999990               0.01000000               0.79500000
           0.10000000               0.00000010               0.19999990

LIGHT KEY= 2            HEAVY KEY= 3
           PLATES ABOVE FEED = 8           PLATES BELOW FEED =10
```

```
ITERATION NUMBER =  1.      SUM OF ABS(1-THETA(I))=   2.78074      C =    1.24464
              I= 1     THETA=  1.931212      XD= 0.2985074     XB= 0.0000000
              I= 2     THETA=  1.004752      XD= 0.6925555     XB= 0.0040014
              I= 3     THETA=  0.698701      XD= 0.0086989     XB= 0.7952335
              I= 4     THETA=  2.543478      XD= 0.0000003     XB= 0.2010047

ITERATION NUMBER =  2.      SUM OF ABS(1-THETA(I))=   0.78053      C =    1.12171
              I= 1     THETA=  1.091275      XD= 0.2985074     XB= 0.0000000
              I= 2     THETA=  1.102487      XD= 0.6933106     XB= 0.0032392
              I= 3     THETA=  0.832932      XD= 0.0081333     XB= 0.7958050
              I= 4     THETA=  1.419696      XD= 0.0000005     XB= 0.2010046

ITERATION NUMBER =  3.      SUM OF ABS(1-THETA(I))=   0.29982      C =    1.06277
              I= 1     THETA=  1.053339      XD= 0.2985075     XB= 0.0000000
              I= 2     THETA=  1.061444      XD= 0.6936730     XB= 0.0028729
              I= 3     THETA=  0.902850      XD= 0.0078073     XB= 0.7961342
              I= 4     THETA=  1.087891      XD= 0.0000006     XB= 0.2010045




ITERATION NUMBER =  4.      SUM OF ABS(1-THETA(I))=   0.12215      C =    1.03228
              I= 1     THETA=  1.031050      XD= 0.2985075     XB= 0.0000000
              I= 2     THETA=  1.034816      XD= 0.6938541     XB= 0.0026902
              I= 3     THETA=  0.947154      XD= 0.0076350     XB= 0.7963080
              I= 4     THETA=  0.996561      XD= 0.0000006     XB= 0.2010045

ITERATION NUMBER =  5.      SUM OF ABS(1-THETA(I))=   0.08593      C =    1.01646
              I= 1     THETA=  1.017385      XD= 0.2985074     XB= 0.0000000
              I= 2     THETA=  1.019102      XD= 0.6939459     XB= 0.0025974
              I= 3     THETA=  0.972109      XD= 0.0075451     XB= 0.7963990
              I= 4     THETA=  0.978452      XD= 0.0000006     XB= 0.2010045
```

```
ITERATION NUMBER =  6.      SUM OF ABS(1-THETA(I))=    0.05382      C =    1.00847
               I= 1     THETA=  1.009633     XD= 0.2985074     XB= 0.0000000
               I= 2     THETA=  1.010298     XD= 0.6939934     XB= 0.0025495
               I= 3     THETA=  0.985388     XD= 0.0074983     XB= 0.7964462
               I= 4     THETA=  0.980728     XD= 0.0000006     XB= 0.2010045

ITERATION NUMBER =  7.      SUM OF ABS(1-THETA(I))=    0.03172      C =    1.00437
               I= 1     THETA=  1.005236     XD= 0.2985074     XB= 0.0000000
               I= 2     THETA=  1.005510     XD= 0.6940179     XB= 0.0025245
               I= 3     THETA=  0.992358     XD= 0.0074737     XB= 0.7964711
               I= 4     THETA=  0.986673     XD= 0.0000006     XB= 0.2010045

ITERATION NUMBER =  8.      SUM OF ABS(1-THETA(I))=    0.01806      C =    1.00229
               I= 1     THETA=  1.002823     XD= 0.2985074     XB= 0.0000000
               I= 2     THETA=  1.002939     XD= 0.6940310     XB= 0.0025115
               I= 3     THETA=  0.995994     XD= 0.0074609     XB= 0.7964839
               I= 4     THETA=  0.991705     XD= 0.0000006     XB= 0.2010045

ITERATION NUMBER =  9.      SUM OF ABS(1-THETA(I))=    0.01006      C =    1.00117
               I= 1     THETA=  1.001513     XD= 0.2985073     XB= 0.0000000
               I= 2     THETA=  1.001565     XD= 0.6940377     XB= 0.0025046
               I= 3     THETA=  0.997896     XD= 0.0074540     XB= 0.7964910
               I= 4     THETA=  0.995120     XD= 0.0000006     XB= 0.2010045

ITERATION NUMBER = 10.      SUM OF ABS(1-THETA(I))=    0.00553      C =    1.00062
               I= 1     THETA=  1.000813     XD= 0.2985074     XB= 0.0000000
               I= 2     THETA=  1.000834     XD= 0.6940414     XB= 0.0025010
               I= 3     THETA=  0.998890     XD= 0.0074504     XB= 0.7964946
               I= 4     THETA=  0.997223     XD= 0.0000006     XB= 0.2010045
```

P

```
THE THIELE GEDDES METHOD HAS CONVERGED
        THE FINAL PLATE COMPOSITICNS ARE...
STEP DOWN COLUMN TO FEED TRAY


PLATE NO=     1          T=  62.293          ITERATIONS=    4.
                   COMPONENT= 1       X= 0.1319054          Y= 0.2985074
                   COMPONENT= 2       X= 0.8450477          Y= 0.6940414
                   COMPONENT= 3       X= 0.0230426          Y= 0.0074504




                   COMPONENT= 4       X= 0.0000043          Y= 0.0000006

PLATE NO=     2          T=  65.437          ITERATIONS=    3.
                   COMPONENT= 1       X= 0.0773953          Y= 0.1914061
                   COMPONENT= 2       X= 0.8740385          Y= 0.7911168
                   COMPONENT= 3       X= 0.0485468          Y= 0.0174739
                   COMPONENT= 4       X= 0.0000200          Y= 0.0000030

PLATE NO=     3          T=  67.083          ITERATIONS=    3.
                   COMPONENT= 1       X= 0.0603727          Y= 0.1563638
                   COMPONENT= 2       X= 0.8505493          Y= 0.8097537
                   COMPONENT= 3       X= 0.0889969          Y= 0.0338695
                   COMPONENT= 4       X= 0.0000817          Y= 0.0000130
```

```
PLATE NO=      4           T=  68.624            ITERATIONS=    3.
                     COMPONENT=  1          X=  0.0537945              Y=  0.1454207
                     COMPONENT=  2          X=  0.7964909              Y=  0.7946535
                     COMPONENT=  3          X=  0.1494033              Y=  0.0598731
                     COMPONENT=  4          X=  0.0003122              Y=  0.0000527

PLATE NO=      5           T=  70.564            ITERATIONS=    3.
                     COMPONENT=  1          X=  0.0495149              Y=  0.1411919
                     COMPONENT=  2          X=  0.7184417              Y=  0.7599017
                     COMPONENT=  3          X=  0.2309353              Y=  0.0987058
                     COMPONENT=  4          X=  0.0011083              Y=  0.0002009

PLATE NO=      6           T=  72.988            ITERATIONS=    3.
                     COMPONENT=  1          X=  0.0454570              Y=  0.1384407
                     COMPONENT=  2          X=  0.6243748              Y=  0.7097272
                     COMPONENT=  3          X=  0.3265632              Y=  0.1511192
                     COMPONENT=  4          X=  0.0036052              Y=  0.0007127

PLATE NO=      7           T=  75.719            ITERATIONS=    3.
                     COMPONENT=  1          X=  0.0414568              Y=  0.1358321
                     COMPONENT=  2          X=  0.5272749              Y=  0.6492556
                     COMPONENT=  3          X=  0.4206206              Y=  0.2125943
                     COMPONENT=  4          X=  0.0106481              Y=  0.0023178

PLATE NO=      8           T=  78.526            ITERATIONS=    3.
                     COMPONENT=  1          X=  0.0377739              Y=  0.1332605
                     COMPONENT=  2          X=  0.4395528              Y=  0.5868343
                     COMPONENT=  3          X=  0.4941456              Y=  0.2730597
                     COMPONENT=  4          X=  0.0285277              Y=  0.0068454
```

```
STEP UP FROM THE REBCILER


PLATE NO=     0          T= 102.364              ITERATIONS=    4.
                     COMPONENT= 1          X= 0.0000000              Y= 0.0000002
                     COMPONENT= 2          X= 0.0025010              Y= 0.0063199
                     COMPONENT= 3          X= 0.7964946              Y= 0.8896388

                     COMPONENT= 4          X= 0.2010045              Y= 0.1040416


PLATE NO=     1          T= 100.745              ITERATIONS=    2.
                     COMPONENT= 1          X= 0.0000001              Y= 0.0000008
                     COMPONENT= 2          X= 0.0053223              Y= 0.0129033
                     COMPONENT= 3          X= 0.8653073              Y= 0.9233857
                     COMPONENT= 4          X= 0.1293705              Y= 0.0637108


PLATE NO=     2          T=  99.886              ITERATIONS=    2.
                     COMPONENT= 1          X= 0.0000006              Y= 0.0000036
                     COMPONENT= 2          X= 0.0101859              Y= 0.0241777
                     COMPONENT= 3          X= 0.8902387              Y= 0.9280221
                     COMPONENT= 4          X= 0.0995751              Y= 0.0477974


PLATE NO=     3          T=  99.256              ITERATIONS=    2.
                     COMPONENT= 1          X= 0.0000026              Y= 0.0000155
                     COMPONENT= 2          X= 0.0185152              Y= 0.0432547
                     COMPONENT= 3          X= 0.8936640              Y= 0.9153770
                     COMPONENT= 4          X= 0.0878187              Y= 0.0413529


PLATE NO=     4          T=  98.512              ITERATIONS=    2.
                     COMPONENT= 1          X= 0.0000115              Y= 0.0000664
                     COMPONENT= 2          X= 0.0326089              Y= 0.0747415
                     COMPONENT= 3          X= 0.8843220              Y= 0.8869688
                     COMPONENT= 4          X= 0.0830576              Y= 0.0382234
```

```
PLATE NO=     5          T=  97.418            ITERATIONS=    2.
                    COMPONENT= 1        X= 0.0000491            Y= 0.0002764
                    COMPONENT= 2        X= 0.0558706            Y= 0.1244851
                    COMPONENT= 3        X= 0.8633347            Y= 0.8393241
                    COMPONENT= 4        X= 0.0807456            Y= 0.0359152

PLATE NO=     6          T=  95.774            ITERATIONS=    2.
                    COMPONENT= 1        X= 0.0002042            Y= 0.0011059
                    COMPONENT= 2        X= 0.0926200            Y= 0.1976768
                    COMPONENT= 3        X= 0.8281360            Y= 0.7678339
                    COMPONENT= 4        X= 0.0790403            Y= 0.0333843

PLATE NO=     7          T=  93.370            ITERATIONS=    3.
                    COMPONENT= 1        X= 0.0008170            Y= 0.0041817
                    COMPONENT= 2        X= 0.1466922            Y= 0.2942678
                    COMPONENT= 3        X= 0.7753207            Y= 0.6713066
                    COMPONENT= 4        X= 0.0771706            Y= 0.0302439

PLATE NO=     8          T=  90.243            ITERATIONS=    3.
                    COMPONENT= 1        X= 0.0030894            Y= 0.0146569
                    COMPONENT= 2        X= 0.2180514            Y= 0.4025711
                    COMPONENT= 3        X= 0.7040086            Y= 0.5562299
                    COMPONENT= 4        X= 0.0748505            Y= 0.0265426

PLATE NO=     9          T=  86.355            ITERATIONS=    3.

                    COMPONENT= 1        X= 0.0108282            Y= 0.0466624
                    COMPONENT= 2        X= 0.2980633            Y= 0.4953339
                    COMPONENT= 3        X= 0.6189926            Y= 0.4354755
                    COMPONENT= 4        X= 0.0721161            Y= 0.0225283
```

```
PLATE NO=    10          T=  81.380          ITERATIONS=    3.
                  COMPONENT= 1        X= 0.0344731             Y= 0.1309499
                  COMPONENT= 2        X= 0.3665943             Y= 0.5306770
                  COMPONENT= 3        X= 0.5297821             Y= 0.3200809
                  CCMPONENT= 4        X= 0.0691504             Y= 0.0182923

ITERATION NUMBER = 11.      SUM OF ABS(1-THETA(I))=    0.00301       C =    1.00034
             I= 1      THETA=  1.000433       XD= 0.2985074      XB= 0.0000000
             I= 2      THETA=  1.000443       XD= 0.6940432      XB= 0.0024991
             I= 3      THETA=  0.999414       XD= 0.0074486      XB= 0.7964965
             I= 4      THETA=  0.998449       XD= 0.0000006      XB= 0.2010045
```

Card Set 4: R,F,D,BTM; Format 4F20.5
Card Set 5: one card per component(I), XF(I),XD(I),XB(I);
Format 3F20.5; no zero values.
Card Set 6: NLK, NHK, NABOVE, NBELOW; Format 4I20

b. Output Data: these are all labeled.

c. IN and IO, the input and output fileset units are read in as DATA.

2. Program Variables: Variable specification, either fixed or floating point, follows standard FORTRAN, unless otherwise specified. The listing for subroutines BUBBLE and DEW is found with CACHE problem "Bubble and Dew Point Calculations with Ideal Mixtures."

A(I), with I .LE. 10, first Antoine constant, component I, for vapor pressure in mm. Hg
ABSUMT, sum of the absolute values of 1 - THETA(I)
AIN(I), input to section A for component I, moles/hr.
AITER, iteration count used in subroutines DEW and BUBBLE
ANCOMP = NCOMP, .LE. 10, the number of components
AOUT(I), output from section A for component I, moles/hr.
ARITER, iteration number for Thiele-Geddes iterative solution
B(I), second Antoine constant for component I, $^{\circ}$K
BIN(I), input to section B for component I, moles/hr.
BL, liquid flow rate down the column below the feed, moles/hr.
BOBL = BTM/BL
BOUT(I), output from section B for component I, moles/hr.
BTM, bottoms flow rate, moles/hr.
C, see Eq. 3
CEXTRA, internal program variable, see card MAIN 132
CONVER, logical variable relating to Thiele-Geddes convergence
D, distillate flow rate, moles/hr.
DFOFC, derivative of FOFC with respect to C
DOV = D/V
F, feed flow rate, moles/hr.
FOFC, function of C used in Newton-Raphson solution for C
FXF(I) = F*XF(I)

NABOVE, the number of plates above the feed tray
NBELOW, the number of plates below the feed tray
NCOMP, the number of components, .LE. 10
NHK, component number of the heavy key
NLK, component number of the light key
NPLATE, the plate number
NSTAGE, the stage number in the stripping section, NPLATE + 1
PI, the total pressure, mm. Hg
PNAME, the problem name, A Format
PSTAR(J), vapor pressure input datum, mm. Hg, corresponding to TPRES(J)
R, reflux ratio
RD, liquid flow rate down the column above the feed, moles/hr.
RDOV = RD/V
T, temperature, °C
TERMS(I), internal program variable, see card MAIN 131
THETA(I), defined by Eq. 2
TK, temperature °K
TOL, tolerance for convergence in subroutines DEW and BUBBLE
TPRES(J), input temperature, °C, corresponding to PSTAR(J)
V, vapor flow rate in the column above the feed, moles/hr.
VB, vapor flow rate in the column below the feed, moles/hr.
VBOBL = VB/BL
X(I), liquid mole fraction, component I
XB(I), bottoms liquid mole fraction, component I
XD(I), distillate liquid mole fraction, component I
XF(I), feed liquid mole fraction, component I
Y(I), vapor mole fraction, component I

3. Program Logic: This is discussed in section II(2) along with the flow chart, Fig. 1.

V. CARD LISTING

See the following pages.

```
$JOB           320505075,KP=29,TIME=60
      C                                                                         MAIN    1
      C     MULTICOMPONENT DISTILLATION RATING CASE                             MAIN    2
      C     USING THE THIELE-GEDDES METHOD                                      MAIN    3
      C     BUBBLE POINT FEED AND REFLUX,  TOTAL CONDENSER,  REBOILER           MAIN    4
      C     NCOMPS=NUMBER OF COMPONENTS,  FLOW RATES IN MOLES/HOUR              MAIN    5
      C     F=FEED,  D= DISTILLATE,  BTM= BOTTOMS FLOW RATES. , R=REFLUX RATIO MAIN    6
      C     RD=R*D= LIQUID FLOW ABOVE FEED, BL= LIQUID FLOW RATE BELOW FEED     MAIN    7
      C     V,VB= VAPOR FLOW RATES ABOVE AND BELOW FEED                         MAIN    8
      C     Y(I),X(I)=VAPOR, LIQUID MOLE FRACTIONS. YOX=Y/X=EQUILIBRIUM K VALUEMAIN    9
      C     NLK,NHK= LIGHT AND HEAVY KEYS..T=DEGREES C, TK= DEGREES K           MAIN   10
      C     PI=TOTAL PRESSURE,TORR.  PSTAR=VAPOR PRESSURE, TORR                 MAIN   11
      C     A,B=ANTOINE CONSTANTS....  LN(PSTAR)=A+B/TK                         MAIN   12
  1          COMMON /POT/X,Y,A,B,T,TK,PI,AITER,NCOMPS,TOL,NPLATE                MAIN   13
  2          LOGICAL CONVER                                                     MAIN   14
  3          DIMENSION X(10),Y(10),A(10),B(10),TPRES(2),PSTAR(2)                MAIN   15
  4          DIMENSION XF(10),XD(10),XB(10)                                     MAIN   16
  5          DIMENSION AIN(10),AOUT(10),BIN(10),BOUT(10),THETA(10)              MAIN   17
  6          DIMENSION PNAME(20),XDOXB(10),FXF(10), TERMS(10)                   MAIN   18
  7          DATA IN,IO/5,6/
      C     PNAME IS THE PROBLEM NAME WRITTEN ON ONE CARD EXCEPT FOR COLUMN ONEMAIN   20
  8        5 READ (IN,109) PNAME                                                MAIN   21
  9          WRITE (IO,110) PNAME                                               MAIN   22
 10      109 FORMAT (20A4)                                                      MAIN   23
 11      110 FORMAT (1H1,20A4)                                                  MAIN   24
      C     READ IN NUMBER OF COMPONENTS,CONSTANT TOTAL PRESSURE,GUESS OF TEMP MAIN   25
      C     OF TOP PLATE, TOLERANCE FOR CONVERGENCE OF DEW AND BUBBLE           MAIN   26
 12          READ (IN,100) ANCOMP, PI, T, TOL                                   MAIN   27
 13      100 FORMAT (4F20.8)                                                    MAIN   28
 14          WRITE (IO,107) ANCOMP,PI,T,TOL                                     MAIN   29
 15      107 FORMAT (//,1X,F5.0,12H COMPONENTS,,5X,15HTOTAL PRESSURE=,F6.0,     MAIN   30
            16H MM HG ,/,5X,38HESTIMATE OF TOP TRAY TEMPERATURE IS    ,F5.0,    MAIN   31
            210H DEGREES C ,/,5X, 49HTOLERANCE ON DEW AND BUBBLE POINT CONVERGEMAIN   32
            3NCE IS       ,F10.5)                                               MAIN   33
 16          NCOMPS=ANCOMP                                                      MAIN   34
 17          IF (NCOMPS .LE.0)STOP                                              MAIN   35
 18          TK=T+273.                                                          MAIN   36
      C        FOR EACH COMPONENT READ IN TWO VAPOR PRESSURES AND TEMPERATURES MAIN   37
      C        AND COMPUTE THE ANTOINE CONSTANTS                                MAIN   38
      WRITE (IO,102)                                                    MAIN  39
  102 FORMAT (//,70H  VAPOR PRESSURE DATA AND ANTOINE CONSTANTS BY COMPOMAIN  40
     1NENT                           )                                  MAIN  41
      DO 90 I=1,NCOMPS                                                  MAIN  42
      READ (IN,100) PSTAR(1),TPRES(1),PSTAR(2),TPRES(2)                 MAIN  43
      B(I)=(ALOG(PSTAR(2))-ALOG(PSTAR(1)))/(1.0/(TPRES(2)+273.0)        MAIN  44
     1-1.0/(TPRES(1)+273.0))                                            MAIN  45
      A(I)=ALOG(PSTAR(1))-B(I)/(TPRES(1)+273.0)                         MAIN  46
   90 WRITE (IO,101) I,PSTAR(1),TPRES(1),PSTAR(2),TPRES(2),A(I),B(I)    MAIN  47
  101 FORMAT (/,3H I=,I1,6X,3HP*=,F10.2,5X,5HAT T=,F10.2,/,10X,3HP*=,   MAIN  48
     1 F10.2,5X,5HAT T=,F10.2,/,10X,2HA=,F15.7,8X,2HB=,F15.7)           MAIN  49
C                                                                       MAIN  50
C     READ IN COLUMN LIQUID FLOW RATES AND REFLUX RATIO                 MAIN  51
      READ (IN,100) R,F,D,BTM                                           MAIN  52
      WRITE (IO,103) R,F,D,BTM                                          MAIN  53
  103 FORMAT (//,14H REFLUX RATIO=,F10.3,10X,5HFEED=,F10.3,10X,         MAIN  54
     111HDISTILLATE=,F10.3,10X,8HBOTTOMS=,F10.3)                        MAIN  55
      WRITE (IO,104)                                                    MAIN  56
  104 FORMAT (//,15X,2HXF,20X,2HXD,20X,2HXB)                            MAIN  57
C    READ IN COMPOSITIONS OF FEED, DISTILLATE, BOTTOMS                  MAIN  58
C     ZERO VALUES OF COMPOSITIONS ARE UNACCEPTABLE                      MAIN  59

      DO 150 I=1,NCOMPS                                                 MAIN  60
      READ (IN,100) XF(I),XD(I),XB(I)                                   MAIN  61
      FXF(I)=F*XF(I)                                                    MAIN  62
      XDOXB(I)=XD(I)/XB(I)                                              MAIN  63
  150 WRITE (IO,100) XF(I),XD(I),XB(I)                                  MAIN  64
C     READ IN THE COMPONENT NUMBER OF THE LIGHT AND HEAVY KEYS          MAIN  65
C     AND NABOVE,NBELOW, THE NUMBER OF PLATES ABOVE AND BELOW THE FEED  MAIN  66
      READ (IN,105) NLK,NHK,NABOVE,NBELOW                               MAIN  67
  105 FORMAT (4I20)                                                     MAIN  68
      WRITE (IO,106) NLK,NHK,NABOVE,NBELOW                              MAIN  69
  106 FORMAT (/,11H LIGHT KEY=,I2,10X,10HHEAVY KEY=,I2,/,10X,           MAIN  70
     119HPLATES ABOVE FEED =,I2,10X,19HPLATES BELOW FEED =,I2)          MAIN  71
C     ADD THE REBOILER AS AN IDEAL STAGE                                MAIN  72
      NBELOW=NBELOW+1                                                   MAIN  73
```

```
C     STARTING CALCULATIONS AT TOP AND INITIALIZATION
      RD=R*D
      V=D+RD
      RDOV=RD/V
      DOV=D/V
C     AFTER CCNVER =.TRUE..ALL THE PLATE COMPOSITIONS ARE PRINTED IN
C     A FINAL PASS THROUGH THE COLUMN
      CCNVER=.FALSE.
      ARITER=0.
  155 ARITER=ARITER+1.
C     SET CCMPOSITION OF TOP PLATE = DISTILLATE COMPOSITION
      DO 160 I=1.NCOMPS
  160 Y(I)=XD(I)
      IF (CONVER) WRITE (IO.170)
  170 FORMAT (30H STEP DOWN COLUMN TO FEED TRAY   ./)
      DO 210 NPLATE=1.NABOVE
  175 CALL DEW
      IF (CONVER) CALL OUT
      DO 210 I=1.NCOMPS
  210 Y(I)=RDOV*X(I)+DOV*XD(I)
C     AT FEED TRAY. CALCULATE AOUT, THE OUTPUT FROM THE UPPER SECTION.A.
C     AND BIN. THE INPUT TO THE LOWER SECTION. B.
      DO 220 I=1.NCOMPS
      AOUT(I)=RD*X(I)+D*XD(I)
  220 BIN(I)=FXF(I)+RD*X(I)
C     INITIALIZE FOR STRIPPING SECTION
      BL=RD+F
      VB=V
      VBOBL=VB/BL
      BOBL=BTM/BL
      DO 280 I=1.NCOMPS
  280 X(I)=XB(I)
      IF (CONVER) WRITE (IO.285)
  285 FORMAT (//.30H STEP UP FROM THE REBOILER       ./)
```

```
      DO 310 NSTAGE=1,NBELOW                                            MAIN 108
      NPLATE=NSTAGE-1                                                   MAIN 109
  290 CALL BUBBLE                                                       MAIN 110
      IF (CONVER) CALL OUT                                              MAIN 111
      DO 310 I=1,NCOMPS                                                 MAIN 112
  310 X(I)=VBOBL*Y(I)+BOBL*XB(I)                                        MAIN 113
      ABSUMT=0.                                                         MAIN 114
C     HAVING CALCULATED UP TO THE FEED TRAY, CALCULATE AIN, THE INPUT TO MAIN 115
C     THE UPPER SECTION,A, AND BOUT, THE OUTPUT FROM THE LOWER SECTION,B.MAIN 116
      DO 320 I=1,NCOMPS                                                 MAIN 117
      AIN(I)=VB*Y(I)                                                    MAIN 118
      BOUT(I)=AIN(I)+BTM*XB(I)                                          MAIN 119



      THETA(I)=(AIN(I)/AOUT(I))*(BOUT(I)/BIN(I))                        MAIN 120
      THETA(I)=SQRT(THETA(I))                                           MAIN 121
C     AOUT(I) SHOULD EQUAL AIN(I), AND BOUT(I) SHOULD EQUAL BIN(I) IF   MAIN 122
C     THE DISTILLATE AND BOTTOMS COMPOSITIONS ARE CORRECT.   THETA(I)   MAIN 123
C     MEASURES THE MISMATCH AND SHOULD CONVERGE TOWARD UNITY.  THETA(I) MAIN 124
C     IS USED TO IMPROVE THE INITIAL ESTIMATES OF XD(I) AND XB(I) AFTER MAIN 125
C     EACH CALCULATION THROUGH THE COLUMN.  THIS IS DONE BY CALCULATING MAIN 126
C     THE NEW RATIO XD/XB=XDOXB(I)=THETA(I)*XD(I)/XB(I).  UNCORRECTED   MAIN 127
C     THIS WOULD GIVE TOP AND BOTTOMS MOLE FRACTIONS WHICH DID NOT SUM TOMAIN 128
C     UNITY.  THE FACTOR C IS ADDED TO FORCE THIS SUM TO UNITY AND C IS MAIN 129
C     FOUND BY A NEWTON-RAPHSON ITERATION WITH AN INITIAL ESTIMATE OF 1. MAIN 130
      TERMS(I)=D*XDOXB(I)*THETA(I)                                      MAIN 131
      CEXTRA=1.0-THETA(I)                                               MAIN 132
C     ABSUMT, THE SUM OF THE DEVIATIONS OF THETA(I) FROM UNITY IS USED  MAIN 133
C     TO DECIDE ON THE CONVERGENCE OF THE COMPOSITIONS THROUGHOUT THE   MAIN 134
C     COLUMN.                                                           MAIN 135
  320 ABSUMT=ABSUMT+ABS(CEXTRA)                                         MAIN 136
```

```
      C=1.0                                                             MAIN 137
  330 FOFC=1.0                                                          MAIN 138
      DFOFC=0.                                                          MAIN 139
      DO 350 I=1,NCOMPS                                                 MAIN 140
      FOFC=FOFC-FXF(I)/(TERMS(I)*C+BTM)                                 MAIN 141
  350 DFOFC=DFOFC+FXF(I)*TERMS(I)/((TERMS(I)*C+BTM)**2)                 MAIN 142
      C=C-FOFC/DFOFC                                                    MAIN 143
      IF(FCFC .GT. 1.0E-5) GO TO 330                                    MAIN 144
      DC 360 I=1,NCOMPS                                                 MAIN 145
      XDOXB(I)=C*THETA(I)*XDOXB(I)                                      MAIN 146
      XB(I)=FXF(I)/(D*XDOXB(I)+BTM)                                     MAIN 147
  360 XD(I)=XB(I)*XDOXB(I)                                              MAIN 148
      WRITE (IO,400) ARITER,ABSUMT,C                                    MAIN 149
  400 FORMAT (//,19H ITERATION NUMBER =,F4.0,5X,23HSUM OF ABS(1-THETA(I)MAIN 150
     1)=,F10.5,5X,3HC =,F10.5)                                          MAIN 151
      WRITE (IO,410) (I,THETA(I),XD(I),XB(I),I=1,NCOMPS)                MAIN 152
  410 FORMAT (15X,2HI=,I2,5X,6HTHETA=,F10.6,5X,3HXD=,F10.7,5X,3HXB=,    MAIN 153
     1F10.7)                                                            MAIN 154
      IF (ARITER .GT. 25) CONVER=.TRUE.                                 MAIN 155
C     THE TCLERANCE ON ABSUMT CAN BE VARIED, BUT 0.01 HAS BEEN FOUND TO MAIN 156
C     BE SATISFACTORY FOR MOST CLASSROOM CALCULATIONS.                  MAIN 157
      IF (ABSUMT .GT. 0.01) GO TO 155                                   MAIN 158
      IF (CCNVER) STOP                                                  MAIN 159
      CCNVER=.TRUE.                                                     MAIN 160
      WRITE (IO,530)                                                    MAIN 161
  530 FORMAT (//,45H THE THIELE GEDDES METHOD HAS CONVERGED        .    MAIN 162
     1/,10X,40HTHE FINAL PLATE COMPOSITIONS ARE...          )           MAIN 163
      GO TC 155                                                         MAIN 164
      END                                                               MAIN 165
      SUBRCUTINE DEW
C     DEW CCMPUTES THE DEW POINT TEMPERATURE AND EQUILIBRIUM LIQUID
C     COMPCSITION FOR A GIVEN VAPOR COMPOSITION
C     THE NEWTON-RAPHSON METHOD IS USED FOR CONVERGENCE TO TOLERANCE TOL
      CCMMCN /POT/X,Y,A,B,T,TK,PI,AITER,NCOMPS,TOL,NPLATE
      DIMENSION X(10),Y(10),A(10),B(10)
      AITER=1.
    1 FOFT=1.
      DFOFT=0.
      DO 2 I=1,NCOMPS
      YCX=(EXP(A(I)+B(I)/TK))/PI
      X(I)=Y(I)/YOX
      FOFT=FUFT-X(I)
    2 DFOFT=DFOFT-X(I)*B(I)/(TK**2)
      IF(ABS(FOFT) .LT. TOL) GO TO 3
      TK=TK-FOFT/DFOFT
      AITER=AITER+1.
      IF (AITER .LT. 15) GO TO 1
    3 SUMX=1.0-FOFT
      DO 4 I=1,NCOMPS
    4 X(I)=X(I)/SUMX
      T=TK-273.
      RETURN
      END
      SUBROUTINE BUBBLE                                                 BUBL   1
C    BUBBLE COMPUTES THE BUBBLE POINT TEMPERATURE AND VAPOR COMPOSITION BUBL   2
C    IN EQUILIBRIUM WITH A GIVEN LIQUID COMPOSITION                     BUBL   3
C    THE NEWTON-RAPHSON METHOD IS USED FOR CONVERGENCE TO TOLERANCE TOL BUBL   4
      COMMON /POT/X,Y,A,B,T,TK,PI,AITER,NCOMPS,TOL,NPLATE               BUBL   5
      DIMENSION X(10),Y(10),A(10),B(10)                                 BUBL   6
      AITER=1.                                                          BUBL   7
   10 FOFT=1.                                                           BUBL   8
      DFOFT=0.                                                          BUBL   9
      DO 20 I=1,NCOMPS                                                  BUBL  10
      YOX=(EXP(A(I)+B(I)/TK))/PI                                        BUBL  11
      Y(I)=YOX*X(I)                                                     BUBL  12
      FOFT=FOFT-Y(I)                                                    BUBL  13
   20 DFOFT=DFOFT+Y(I)*B(I)/(TK**2)                                     BUBL  14
      IF (ABS(FOFT).LT.TOL)GO TO 30                                     BUBL  15
      TK=TK-FOFT/DFOFT                                                  BUBL  16
      AITER=AITER+1.                                                    BUBL  17
      IF (AITER .LT. 15) GO TO 10                                       BUBL  18
   30  SUMY=1.0-FOFT                                                    BUBL  19
      DO 40 I=1,NCOMPS                                                  BUBL  20
   40 Y(I)=Y(I)/SUMY                                                    BUBL  21
      T=TK-273.                                                         BUBL  22
      RETURN                                                            BUBL  23
      END                                                               BUBL  24

      SUBROUTINE OUT                                                    OUT    1
C                                                                       OUT    2
C    OUT PRINTS THE PLATE TEMPERATURE AND COMPOSITION                   OUT    3
      COMMON /POT/X,Y,A,B,T,TK,PI,AITER,NCOMPS,TOL,NPLATE               OUT    4
      DIMENSION X(10),Y(10),A(10),B(10)                                 OUT    5
      DATA IO/6/
      WRITE (IO,180) NPLATE,T,AITER                                     OUT    7
  180 FORMAT (//,10H PLATE NO=,I5,10X,2HT=,F8.3,10X,11HITERATIONS=,F5.0)OUT    8
      DO 190 I=1,NCOMPS                                                 OUT    9
  190 WRITE (IO,200) I,X(I),Y(I)                                        OUT   10
  200 FORMAT (20X,11H COMPONENT=,I2,7X,2HX=,F10.7,10X,2HY=,F10.7)       OUT   11
      RETURN                                                            OUT   12
      END                                                               OUT   13
```

I. PROBLEM IDENTIFICATION

1. Title: Equilibrium Separation in a Multicomponent Multicolumn System
2. Author: John W. Tierney
3. Affiliation: University of Pittsburgh

II. TECHNICAL DESCRIPTION

1. Problem Statement: A distillation system consisting of two columns is shown schematically in Figure 1. Feed enters column one, and a vapor product is produced from stage 1 and a liquid product from stage 5. A portion of the liquid leaving stage 3 is used as feed to the second column, which produces a liquid product from stage 7. Vapor is returned to the main column at stage 2. The direction of the flows between stages is indicated by the arrows--an arrow pointing upward is a vapor flow, and an arrow pointing down is a liquid flow.

Given all the vapor flows: find the liquid flows, the temperatures in each stage, and the compositions in each stage. Assume that the liquid and vapor phases in each stage are at equilibrium. It will be necessary to use the material balance equations and the equilibrium relations. Energy balance equations will not be needed. This problem can, however, be considered as part of a larger problem in which the vapor flows are varied in such a way as to satisfy the energy balance equations.

a. Calculation of liquid flow rates: Given the set of vapor flow rates, calculate the liquid flow rates using the overall material balance equation.

Data: All feed enters stage 4. The feed rate is 80 kg moles/hr and consists of three components.

Component	1 isobutane	2 n butane	3 neo pentane
Flow rate (kg moles/hr)	40.0	20.0	20.0

The total vapor flow leaving each stage is to be:

Stage	1	2	3	4	5	6	7
Rate (kg moles/hr)	40.0	160.0	120.0	120.0	40.0	40.0	40.0

These flows are also indicated on the flow diagram. Half of the liquid leaving stage 3 goes to stage 6 and half to stage 4.

b. Calculation of stage compositions: Using the temperatures specified below calculate all phase compositions assuming equilibrium in each stage and using the component material balance equations. Also calculate the error in the sum of compositions for each stage.

Data: For the first calculation of stage compositions, assume the stage temperatures are as follows. These temperatures will be corrected in Part c.

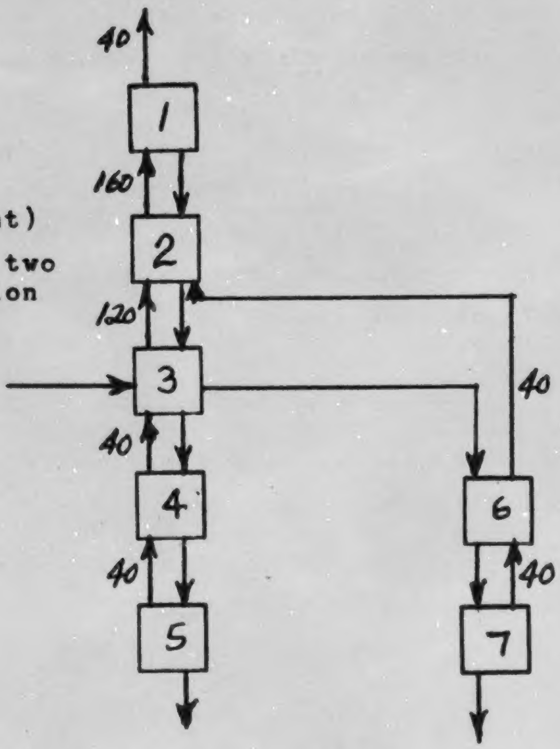
Stage	1	2	3	4	5	6	7
Temperature (°C)	39	42	45	48	51	46	48

The pressure is 5 atm in all stages. Equilibrium ratios can be obtained by using Raoult's law if other data are not available.

c. Correction of temperatures: Use the "bubble point method" to correct the temperatures assumed in Part b. Repeat this procedure until the Euclidean norm of the composition errors (defined by Equation (5) in Section 3) is less than 0.01.

FIGURE 1 (at right)

Flow diagram for two column distillation system.



2. Problem Formulation and Technical Analysis: The solution of multistage equilibrium separation problems requires the solution of large sets of simultaneous equations. With 7 stages and 3 components as in this problem, there are 7 overall material balances, 21 component material balances, 21 equilibrium relations, and 7 sum of composition requirements. Matrix notation is used to simplify writing the equations and is particularly advantageous in a multicolumn problem where the interstage flow patterns are not strictly countercurrent. The columns are not treated separately in this analysis but are solved simultaneously.

In Part a, only the overall material balances are solved. This requires the solution of a set of 7 linear simultaneous equations.

In Part b, a temperature is assumed for each stage and the liquid and vapor compositions are calculated. There are a total of 42 simultaneous equations to be solved, but they can very conveniently be solved as three sets of 14 simultaneous equations, one for each component.

The compositions calculated in Part b do not satisfy the requirement that the liquid and vapor mole fractions sum to 1.0 in each stage because the assumed temperatures were not correct.

In Part c the 7 errors in sums of compositions are used to correct the 7 temperatures, and the calculation is repeated until the errors are reduced to an acceptable level.

3. Method of Solution: The matrix notation proposed in references 1-4 is used. All variables are defined in the next section.

For Part a, the $\underset{\sim}{A}$, $\underset{\sim}{B}$, and $\underset{\sim}{F}$ matrices must be correctly formulated from the problem statement. The correct values are listed in the computer output for the problem. The only entries which might cause difficulty are the two values of 0.5 in column 3 of $\underset{\sim}{B}$. These are needed because one-half the liquid leaving stage 3 goes to stage 4 and one-half goes to stage 6. The liquid flow vector, L, is obtained by solving the set of simultaneous linear equations,

$$\underset{\sim}{B}\, L = -\left(\underset{\sim}{A}\, V + \sum_{j=1}^{m} (F^j)\right) \qquad (1)$$

This equation is an overall material balance for all stages.

For Part b, the stage temperatures and pressures are given. The equilibrium ratios can then be calculated for each component in each stage. The equilibrium equation in matrix form is given by,

$$Y^j = \underset{\sim}{K}^j\, X^j \qquad 1 \leq j \leq m \qquad (2)$$

The component material balance for each component is given by

$$\underset{\sim}{A}\, \underset{\sim}{V}\, Y^j + \underset{\sim}{B}\, \underset{\sim}{L}\, X^j + F^j = 0 \qquad (3)$$

It should be noted that $\underset{\sim}{V}$ and $\underset{\sim}{L}$ are diagonal matrices with the same elements on the diagonal as the vectors V and L. The vapor compositions can be eliminated between Equations 2 and 3 to give

$$(\underset{\sim}{A}\, \underset{\sim}{V}\, \underset{\sim}{K}^j + \underset{\sim}{B}\, \underset{\sim}{L})\, X^j = -F^j \qquad 1 \leq j \leq m \qquad (4)$$

All variables are known except X^j, and therefore this is a set of simultaneous linear equations in the liquid compositions for component j. These are solved for each component. The vapor compositions are calculated using Equation (2).

Because the assumed temperatures are not correct, the mole fractions in each stage will not sum to 1.0. The error in the sum of compositions in each stage is defined as the difference between the sum of the liquid compositions and the sum of the vapor compositions.

$$d_i = \sum_{j=1}^{m} (x_{ij}) - \sum_{j=1}^{m} (y_{ij}) \qquad 1 \leq i \leq n \qquad (5)$$

In Part c the error in the sum of compositions for each stage is used to correct the temperature for the stage. The "bubble point" correction method is used, and the new temperature for stage i is given by

$$(t_i)_{k+1} = (t_i)_k - (d_i)_k/(e_i)_k \qquad 1 \leq i \leq n \qquad (6)$$

where the correction factor e_i is defined as,

$$(e_i) = - \sum_{j=1}^{m} \{(x_{ij})(\frac{dk_{ij}}{dt_i})\} \qquad 1 \le i \le n \qquad (7)$$

4. References and Data:

References

1. Tierney, J. W. and J. A. Bruno, "Equilibrium Stage Calculations," AIChE Journal, 1967, 13, p. 556.

2. Tierney, J. W. and J. L. Yanosik, "Simultaneous Flow and Temperature Corrections in the Equilibrium Stage Problem," AIChE Journal, 1969, 15, p. 897.

3. Tierney, J. W. Yanosik, J. L., and Bruno, J. A., "Solution of Equilibrium Stage Models for Solvent Extraction Processes," Proceedings International Solvent Extraction Conference 1971, pp. 1051-1061, Society of Chemical Industry, London (1971).

4. Bruno, J. A., J. L. Yanosik, and J. W. Tierney, "Distillation Calculations with Nonideal Mixtures," presented to American Chemical Society, Boston, April, 1972.

Notation

$\underset{\sim}{A}$	Vapor recycle matrix (n x n). Diagonal elements are -1. Element ij ($i \neq j$) is the fraction of the total vapor leaving stage j which goes to stage i.
$\underset{\sim}{B}$	Liquid recycle matrix (n x n). Diagonal elements are -1. Element ij is fraction of total liquid leaving stage j that goes to stage i.
D	Error vector (n). Element i defined by equation 5.
E	Correction vector (n). Element i is defined by equation 7.
$\underset{\sim}{F}$	Feed matrix (n x m). Element ij is amount of component j entering stage i as feed per unit time.
F^j	Component feed vector (n). Column j of F.
$\underset{\sim}{K}^j$	Equilibrium ratio matrix (n x n). Diagonal. Element ii is equilibrium ratio for component j in stage i.
L	Liquid flow vector (n). Element i is total amount of liquid leaving stage i per unit time.
$\underset{\sim}{L}$	Liquid flow matrix (n x n). Diagonal. Non-zero elements are the same as in vector L.
m	Scalar. Number of components.
n	Scalar. Number of stages.

T	Temperature vector (n). Element i is temperature in stage i.
V	Vapor flow vector (n). Element i is total amount of vapor leaving stage i per unit time.
$\underset{\sim}{V}$	Vapor flow matrix (n x n). Diagonal. Non-zero elements the same as those in vector V.
X^j	Liquid composition vector (n). Element i is mole fraction of component j in liquid in stage i.
Y^j	Vapor composition vector (n). Element i is mole fraction of component j in the vapor in stage i.

5. Solution:

a. Results: A computer program to solve this problem is given in the following pages. The program makes use of the matrix handling subroutines found in the Scientific Subroutine Package for FORTRAN. Subroutines which are needed for the program but not listed with the program are briefly described below. In the arguments for each subroutine, the following standard notation is used.

A single letter is the name of a matrix or vector.

NRA is number of rows of matrix A.

NCA is the number of columns of matrix A.

MA is the mode of storage of matrix A. If a 0 is used, the matrix is general; i.e., all elements are stored. If this argument is a 2, the matrix is diagonal, and only the diagonal elements are stored.

CADD(A,ICA,B,ICB,NRA,NCA,MA,NCB) Column ICA of matrix A is added to column ICB of matrix B.

CCPY(A,ICA,B,NRA,NCA,MA) Column ICA of matrix A is copied to vector B.

GELG(A,B,NRA,NCA,EPS,IER) The simultaneous equations B X = A are solved, with the answer being placed in A. EPS is a relative tolerance and IER is set to 0 if the equations are successfully solved.

MADD(A,B,C,NRA,NCA,MA,MB) Matrix A is added to matrix B and the sum placed in matrix C.

MCPY(A,B,NRA,NCA,MA) Matrix A is copied into matrix B.

MPRD(A,B,C,NRA,NCA,MA,MB,NCB) The product of matrix A and B is placed in matrix C.

MSUB(A,B,C,NRA,NCA,MA,MB) Matrix B is subtracted from matrix A and the difference placed in matrix C.

RSUM(A,B,NRA,NCA,MA) The rows of matrix A are summed and placed in vector B.

SCLA(A,S,NRA,NCA,MA) Each element of the matrix A is set equal to the scalar S.

SMPY(A,S,B,NRA,NCA,MA) The product of the matrix A and the scalar S is put in the matrix B.

b. Discussion of Results: Computer output for the sample problem is given after the program listing. Three iterations were needed to satisfy the convergence criterion specified in the problems. Liquid and vapor compositions are given and the product compositions and amounts can be readily determined.

III. EDUCATIONAL (PEDOGOLOGICAL) ASPECTS

1. Description of Past Usage: This problem or a variation has been used at two levels. At the sophomore level, a version of the program in BASIC language is available at a remote terminal, and each student must modify the program to solve his problem - change the flow pattern, number of stages, product withdrawals, etc. This is one home problem assignment, and can be done in two or three days, depending on the availability of terminals.

At the upper class or first year graduate student level, the student is asked to write the complete program. This requires about two weeks.

2. Concepts Demonstrated: Equilibrium stage separation principles, material balances, solution of sets of simultaneous equations.

3. Evaluation of Usage: At the first level - program modification - students have little difficulty in obtaining a solution. By giving each student in a class a slightly different problem the effect of changing column parameters can be demonstrated.

When asked to write a complete program, not all students will be successful. Most will finish Part a and be well along on the remainder of the problem - the major difficulties being the usual programming bugs such as FORMAT mistakes. Those who finish gain real confidence and insight into solution methods for equilibrium separations problems.

4. Program Description: The program presented below is intended as an example of a good program a student might write. It is not intended as a general program for production use. It will solve only the example problem described above, but it can readily be modified to solve other problems by making the changes listed below. For student use, this is generally desirable because the student is more likely to study the program and understand its operation.

For a problem with n stages and m components;

Matrices A,B,WA,WB, and WC should be dimensioned to n by n.

Matrices X,Y, and F should be dimensioned to n by m.

The dimensions of vectors V,FL,P,T,UA, and UB, and UC must be n or larger.

Vectors CA and CB in functions ER and DER must be m or larger.

The program structure is straightforward, following almost exactly the sequence of calculations given above in II-3. Matrix manipulations are done with subroutines from the FORTRAN Scientific Subroutine Package, and a listing of the subroutines with their arguments is given above in II-5. Any computation center should have this set of subroutines or their equivalent available. One other subroutine and two functions are used. The subroutine MWRT is used for output of matrices and vectors. The function ER returns the equilibrium ratio for a component, and function DER returns the derivative with respect to temperature of the equilibrium ratio. Very simple equations are used for the equilibrium ratio calculation, and better equations can be used when available. A description of the programs follows:

MAIN: This program calls on subroutines from the Scientific Subroutine Package, the output subroutine MWRT, and function ER and DER. All input is by means of DATA statements. The variables are:

A	Vapor flow distribution matrix
B	Liquid flow distribution matrix
DNORM	Euclidean norm of error vector
E	Error in stage sum of compositions
F	Feed matrix
FL	Liquid flow vector, called L in equations
ITER	Counter for number of iterations
IOUT	Number of output device
P	Stage pressure vector
T	Stage temperature vector
UA,UB,UC	Vectors used for temporary storage
WA,WB,WC	Matrices used for temporary storage
X	Liquid composition matrix
Y	Vapor composition matrix

MWRT(A,N,M,IOUT): This subroutine prints a matrix by rows, 10 elements per line. The format F12.4 is used. A vector is printed as a row. The arguments are:

A	The name of the matrix
N	The number of rows to be printed, integer
M	The number of columns to be printed, integer. If A is a vector, N should be 1
IOUT	The number of the output device, integer

ER(J,T,P): Function subprogram for calculating the equilibrium ratio by dividing the vapor pressure of the pure component by the total pressure. The vapor pressure is assumed equal to exp(a/t + b) where a and b are constants which are different for each component. The arguments are:

J	Component number, integer
T	Stage temperature
P	Stage pressure

The constants for the vapor pressure equation must be entered in the vectors CA and CB through DATA statements.

DER(J,T,P): Function subprogram for calculating the derivative of the equilibrium ratio with respect to temperature. The derivative is given by $k(-a/t^2)$ where k is the equilibrium ratio. This subprogram calls on ER for the equilibrium ratio. The arguments are the same as in ER. The constants CA are entered by a DATA statement and are the same as in ER.

V. PROGRAM DESCRIPTION

```
C      MAIN                                                              MAIN0010
C      THIS PROGRAM IS A SOLUTION TO THE MULTICOMPONENT, MULTCOLUMN      MAIN0020
C      DISTILLATION PROBLEM IN WHICH THE FLOWS ARE FIXED.  TEMPERATURES  MAIN0030
C      ARE CORRECTED BY A BUBBLE POINT METHOD.  FLOWS ARE FIXED.         MAIN0040
C      ENERGY BALANCES ARE NOT INCLUDED                                  MAIN0050
C      SOLUTION IS DIVIDED INTO THREE PARTS                              MAIN0060
C*****PART1.- THE LIQUID FLOW RATE VECTOR IS CALCULATED FOR A GIVEN      MAIN0070
C        VAPOR FLOW RATE VECTOR                                          MAIN0080
C                                                                        MAIN0090
C        IMPORTANT VARIABLES                                             MAIN0100
C             M NUMBER OF COMPONENTS                                     MAIN0110
C             N NUMBER OF STAGES                                         MAIN0120
C             A VAPOR FLOW DISTRIBUTION MATRIX                           MAIN0130
C             B  LIQUID FLOW DISTRIBUTION MATRIX                         MAIN0140
C             F  FEED MATRIX                                             MAIN0150
C             V  VAPOR FLOW RATE VECTOR                                  MAIN0160
C             FL  LIQUID FLOW RATE VECTOR                                MAIN0170
C             UA, UB, UC, WA ARE USED FOR TEMPORARY STORAGE              MAIN0180
C      MATRICES ARE DIMENSIONED FOR A PROBLEM WITH 7 STAGES AND 3        MAIN0190
C      COMPONENTS.  MATRIX DIMENSIONS MUST BE CHANGED IF PROBLEM SIZE    MAIN0200
C      IS CHANGED.                                                       MAIN0210
       DIMENSION A(7,7), B(7,7), F(7,3), WA(7,7)                         MAIN0220
      1 FL(25), V(25), UA(25),  UB(25),  UC(25)                          MAIN0230
       DIMENSION X(7,3), Y(7,3), WB(7,7), WC(7,7), T(25), P(25)          MAIN0235
C      INPUT DATA                                                        MAIN0240
C                                                                        MAIN0250
C      DATA STATEMENTS ARE USED FOR ALL INPUT                            MAIN0260
C                                                                        MAIN0270
C      ELEMENTS OF MATRIX A ARE ENTERED BY COLUMNS                       MAIN0280
       DATA A/-1.,6*0., 1.,-1.,6*0.,  1.,-1., 6*0., 1., -1., 6*0.,       MAIN0290
      1 1., -1., 3*0., 1., 3*0., -1.,6*0., 1., -1./,                     MAIN0300
C      ELEMENTS OF MATRIX B ARE ENTERED BY COLUMNS                       MAIN0310
      2 B/-1., 1., 6*0., -1.,1., 6*0., -1.,0.5, 0.0, 0.5, 4*0.0,         MAIN0320
      3 -1., 1., 6*0., -1., 7*0., -1., 1., 6*0., -1./                    MAIN0330
```

```
C      ELEMENTS OF FEED MATRIX F ARE ENTERED BY COLUMNS                  MAIN0340
       DATA F/3*0.,40.,6*0.,20.,6*0.,20.,3*0./                           MAIN0350
C      ELEMENTS OF VAPOR FLOW RATE VECTOR ARE ENTERED                    MAIN0360
       DATA V/40., 160., 120., 120.,40.,40.,40.,18*0./                   MAIN0370
C      NUMBER OF STAGES, NUMBER OF COMPONENTS, NUMBER OF OUTPUT DEVICE   MAIN0380
       DATA N/7/, M/3/,IOUT/6/                                           MAIN0390
C      INPUT DATA IS ECHOED                                              MAIN0400
       WRITE(IOUT,100)                                                   MAIN0410
   100 FORMAT(1H1,15H***MATRIX A*** )                                    MAIN0420
       CALL MWRT(A,N,N,IOUT)                                             MAIN0430
       WRITE(IOUT,110)                                                   MAIN0440
   110 FORMAT(1H0,15H***MATRIX B*** )                                    MAIN0450
       CALL MWRT(B,N,N,IOUT)                                             MAIN0460
       WRITE (IOUT,115)                                                  MAIN0462
   115 FORMAT(1H0,17H***FEED MATRIX*** )                                 MAIN0465
       CALL MWRT(F,N,M,IOUT)                                             MAIN0467
       WRITE(IOUT,120)                                                   MAIN0470
   120 FORMAT(1H0,23H***VAPOR FLOW VECTOR*** )                           MAIN0480
       CALL MWRT(V,N,1,IOUT)                                             MAIN0490
C      THE FEED COLUMN VECTORS ARE SUMMED AND ADDED TO (A*V)             MAIN0500
       CALL RSUM(F,UB,N,M,0)                                             MAIN0510
   300 CALL MPRD(A,V,UA,N,N,0,0,1)                                       MAIN0520
       CALL MADD(UA,UB,UC,N,1,0,0)                                       MAIN0530
C      THE SUM IS NEGATED                                                MAIN0540
       CALL SMPY(UC,-1.,UA,N,1,0)                                        MAIN0550

C      THE LIQUID FLOW RATES ARE CALCULATED                              MAIN0560
       CALL MCPY(B,WA,N,N,0)                                             MAIN0570
       CALL GELG(UA,WA,N,1,1.E-6,IER)                                    MAIN0580
       CALL MCPY(UA,FL,N,1,0)                                            MAIN0590
C      THE CALCULATED FLOW RATES ARE PRINTED                             MAIN0600
       WRITE(IOUT,310)                                                   MAIN0610
   310 FORMAT(1H0,24H***LIQUID FLOW VECTOR*** )                          MAIN0620
       CALL MWRT(FL,N,1,IOUT)                                            MAIN0630
```

```
                                                                        MAIN0640
C                                                                       MAIN0650
C*****PART 2 OF PROBLEM.                                                MAIN0660
C     FOR AN ASSUMED TEMPERATURE VECTOR THE STAGE COMPOSITIONS ARE      MAIN0670
C     CALCULATED AND THE ERROR IN THE SUM OF COMPOSITIONS IS            MAIN0680
C     DETERMINED                                                        MAIN0690
C     NEW VARIABLES                                                     MAIN0700
C           X  LIQUID COMPOSITION MATRIX                                MAIN0710
C           Y  VAPOR COMPOSITION MATRIX                                 MAIN0720
C           T  TEMPERATURE VECTOR                                       MAIN0730
C           P  PRESSURE VECTOR                                          MAIN0740
C           WB AND WC ARE USED FOR TEMPORARY STORAGE                    MAIN0750
C                                                                       MAIN0760
C     MATRIX DIMENSIONS MUST BE CHANGED IF PROBLEM SIZE IS CHANGED      MAIN0770
C                                                                       MAIN0780
C                                                                       MAIN0790
C     STAGE TEMPERATURES IN DEGREES CENTIGRADE                          MAIN0800
      DATA T/39.,42.,45.,48.,51.,46.,48.,18*0./                         MAIN0810
C     STAGE PRESSURES IN ATMOSPHERES                                    MAIN0820
      DATA P/5.,5.,5.,5.,5.,5.,5.,18*0./                                MAIN0830
C     START A COUNTER FOR THE NUMBER OF ITERATIONS                      MAIN0840
      ITER=1                                                            MAIN0850
C     CLEAR X AND Y MATRICES                                            MAIN0860
  400 CALL SCLA(X,0.,N,M,0)                                             MAIN0870
      CALL SCLA(Y,0.,N,M,0)                                             MAIN0880
C     HEADING FOR OUTPUT                                                MAIN0890
      WRITE(IOUT,410) ITER                                              MAIN0900
  410 FORMAT(1H1,27H*****RESULTS FOR ITERATION ,I3,16H BEGIN HERE*****) MAIN0910
      WRITE(IOUT,420)                                                   MAIN0920
  420 FORMAT(1H0,30H**ASSUMED TEMPERATURE VECTOR**)                     MAIN0930
      CALL MWRT(T,N,1,IOUT)                                             MAIN0940
C                                                                       MAIN0950
C     COMPOSITIONS ARE CALCULATED FOR EACH COMPONENT                    MAIN0960
  430 DO 600 J=1,M                                                      MAIN0970
C     EQUILIBRIUM RATIOS ARE CALCULATED AND PUT IN UC FOR COMPONENT J   MAIN0980
      DO 500 I=1,N                                                      MAIN0990
  500 UC(I)=ER(J,T(I),P(I))
```

```
      CALL MPRD(V,UC,WB,N,N,2,2,N)                                      MAIN1000
      CALL MPRD(A,WB,WC,N,N,0,2,N)                                      MAIN1010
      CALL MPRD(B,FL,WB,N,N,0,2,N)                                      MAIN1020
      CALL MADD(WB,WC,WB,N,N,0,0)                                       MAIN1030
      CALL CCPY(F,J,UA,N,M,0)                                           MAIN1040
      CALL SMPY(UA,-1.,UA,N,1,0)                                        MAIN1050
C     SIMULTANEOUS EQUATIONS ARE SOLVED FOR LIQUID COMPOSITION OF J     MAIN1060
      CALL GELG(UA,WB,N,1,1.E-6,IER)                                    MAIN1070
      CALL CADD(UA,1,X,J,N,1,0,M)                                       MAIN1080
C     VAPOR PHASE COMPOSITIONS ARE CALCULATED FOR COMPONENT J           MAIN1090
      CALL MPRD(UC,UA,UB,N,N,2,0,1)                                     MAIN1100
      CALL CADD(UB,1,Y,J,N,1,0,M)                                       MAIN1110
  600 CONTINUE                                                          MAIN1120
C     LIQUID AND VAPOR PHASE COMPOSITIONS ARE PRINTED                   MAIN1130
      WRITE(IOUT,610)                                                   MAIN1140
  610 FORMAT(1H0,30H**LIQUID COMPOSITION MATRIX**    )                  MAIN1150
      CALL MWRT(X,N,M,IOUT)                                             MAIN1160
      WRITE(IOUT,620)                                                   MAIN1170
  620 FORMAT(1H0,28H**VAPOR COMPOSITION MATRIX**)                       MAIN1180
      CALL MWRT(Y,N,M,IOUT)                                             MAIN1190
C     LIQUID AND VAPOR COMPOSITIONS ARE SUMMED FOR EACH STAGE           MAIN1200
      CALL RSUM(X,UA,N,M,0)                                             MAIN1210
      CALL RSUM(Y,UB,N,M,0)                                             MAIN1220
      CALL MSUB(UA,UB,UC,N,1,0,0)                                       MAIN1230
C     ERRORS IN SUM OF COMPOSITIONS FOR EACH STAGE ARE PRINTED          MAIN1240
      WRITE(IOUT,630)                                                   MAIN1250
  630 FORMAT(1H0,37H**MATERIAL BALANCE ERROR VECTOR IS** )              MAIN1260
      CALL MWRT(UC,N,1,IOUT)                                            MAIN1270
C     THE NORM OF THE ERROR VECTOR IS CALCULATED                        MAIN1280
      DNORM=0                                                           MAIN1290
      DO 700 IJ=1,N                                                     MAIN1300
  700 DNORM=DNORM+UC(IJ)*UC(IJ)                                         MAIN1310
      DNORM=SQRT(DNORM)                                                 MAIN1320
      WRITE(IOUT,710) (DNORM)                                           MAIN1330
  710 FORMAT(1H0,32H**MATERIAL BALANCE ERROR NORM IS ,E15.5,2H**)       MAIN1340
```

```
C                                                                         MAIN1350
C*****PART 3.  TEMFERATLRES ARE CORRECTEC USING A BUEBLE POINT METHCD     MAIN1360
C                                                                         MAIN1370
C      IF THE ERROR NCRM IS LESS THAN 0.01. A SCLUTION HAS BEEN OBTAINED MAIN1380
       IF (CNCRM.LE.0.01) GC TO 1000                                      MAIN1390
C      IF MCRE THAN 10 ITERATIONS ARE REQUIRED IT IS ASSUMED THAT         MAIN1400
C      THE SEGUENCE IS DIVERGENT AND CALCULATICNS ARE TERMINATED          MAIN1410
       IF (ITER.GE.10) GC TC 1100                                         MAIN1420
C       TEMFERATURES ARE CCRRECTED ONE STAGE AT A TIME                    MAIN1430
       DC 8C0 I=1.N                                                       MAIN1440
       E=0.                                                               MAIN1450
       DC 750 J=1,M                                                       MAIN1460
  750 E=E-X(I,J)*DER(J,T(I),P(I))                                         MAIN1470
  800 T(I)=T(I)-UC(I)/E                                                   MAIN1480
C      CCRRECTED TEMPERATURES ARE PRINTED                                 MAIN1490
       WRITE(IOUT,810)                                                    MAIN1500
  810 FCRMAT(1H0,32H**CCRRECTED TEMPERATURE VECTOR**)                     MAIN1510
       CALL MWRT(T,N,1,ICUT)                                              MAIN1520
C      ITERATION NUMBER INCREASED BY ONE AND CALCULATICNS REPEATED        MAIN1530
       ITER=ITER+1                                                        MAIN1540
         GC TC 400                                                        MAIN1550
C      MESSAGE FCR A SUCCESSFLL TERMINATION IS PRINTED                    MAIN1560
 1000 WRITE(IOUT,1010)                                                    MAIN1570
 1010 FCRMAT (1H0,34H******CALCULATION TERMINATED****** ./  .1H  .        MAIN1580
     137H******ERRCR NORM LESS THAN 0.01******)                           MAIN1590
       GC TC 1200                                                         MAIN1600
C      MESSAGE FCR AN UNSUCESSFUL TERMINATION IS PRINTED                  MAIN1610
 1100 WRITE(IOUT,1110)                                                    MAIN1620
 1110 FCRMAT(1H0, 34H******CALCULATION TERMINATED****** ./.1H  .          MAIN1630
     136H******MORE THAN 10 ITERATIONS******  )                           MAIN1640
 1200 STCP                                                                MAIN1650
       END                                                                MAIN1660
```

```
C     MWRT                                                              MWRT0010
C     SUBROUTINE TO PRINT A MATRIX BY ROWS.                             MWRT0020
C     MATRIX A WITH N ROWS AND M COLUMNS IS PRINTED BY ROWS,TEN         MWRT0030
C     ELEMENTS TO A LINE USING THE FORMAT F12.4                         MWRT0040

      SUBROUTINE MWRT(A,N,M,IOUT)                                       MWRT0050
      DIMENSION A(N,M),B(10)                                            MWRT0060
C     A ONE COLUMN MATRIX WILL BE PRINTED AS A ROW VECTOR               MWRT0070
      IF (M.EQ.1) GO TO 120                                             MWRT0080

      DO 100 I=1,N                                                      MWRT0090
      DO 90 J=1,M                                                       MWRT0100
   90 B(J)=A(I,J)                                                       MWRT0110
  100 WRITE(IOUT,110)(B(J),J=1,M)                                       MWRT0120
  110 FORMAT(1H ,10F12.4,/)                                             MWRT0130
      GO TO 140                                                         MWRT0140
  120 WRITE(IOUT,110)(A(I,1),I=1,N)                                     MWRT0150
  140 RETURN                                                            MWRT0160
      END                                                               MWRT0170
```

```
              C       DER                                                               DER 0010
              C                                                                         DER 0020
              C       FUNCTION SUBPROGRAM TO CALCULATE DERIVATIVE OF EQUILIBRIUM RATIO  DER 0030
 0001                 REAL FUNCTION DER(J,T,P)                                          DER 0040
              C       J IS COMPONENT NUMBER, T IS TEMPERATURE IN DEGREES CENTIGRADE     DER 0050
              C       P IS PRESSURE IN ATMOSPHERES                                      DER 0060
 0002                 DIMENSION CA(3)                                                   DER 0070
              C       COMPONENT 1 IS ISOBUTANE, 2 IS N-BUTANE, 3 IS NEO PENTANE         DER 0080
 0003                 DATA CA/-2549.17, -2771.61, -2934.24/                             DER 0090
 0004                 DER=ER(J,T,P)*(-CA(J)/(T+273.2)**2)                               DER 0100
 0005                 RETURN                                                            DER 0110
 0006                 END                                                               DER 0120
```

```
              C       ER                                                                ER  0010
              C       FUNCTION SUBPROGRAM TO CALCULATE EQUILIBRIUM RATIOS               ER  0020
              C       VAPOR PRESSURE FOR PURE COMPONENT IS DIVIDED BY TOTAL PRESSURE    ER  0030
              C       VAPOR PRESSURES CALCULATED BY P=EXP(A/T+B)                        ER  0040
 0001                 REAL FUNCTION ER(J,T,P)                                           ER  0050
              C       J IS COMPONENT NUMBER, T IS TEMPERATURE IN DEGREES CENTIGRADE     ER  0060
              C       P IS PRESSURE IN ATMOSPHERES                                      ER  0070
 0002                 DIMENSION CA(3),CB(3)                                             ER  0080
              C       CA AND CB ARE CONSTANTS A AND B IN VAPOR PRESSURE EQUATION        ER  0090
              C       COMPONENT 1 IS ISOBUTANE, 2 IS N-BUTANE, 3 IS NEO PENTANE         ER  0100
 0003                 DATA CA/-2549.17, -2771.61, -2934.24/                             ER  0110
 0004                 DATA CB/9.7746, 10.1850, 10.3867/                                 ER  0120
 0005                 ER=(1./P)*EXP(CA(J)/(T+273.2)+CB(J))                              ER  0130
 0006                 RETURN                                                            ER  0140
 0007                 END                                                               ER  0150
```

```
***MATRIX A***
     -1.0000      1.0000         0.0         0.0         0.0         0.0         0.0
         0.0     -1.0000      1.0000         0.0         0.0      1.0000         0.0
         0.0         0.0     -1.0000      1.0000         0.0         0.0         0.0
         0.0         0.0         0.0     -1.0000      1.0000         0.0         0.0
         0.0         0.0         0.0         0.0     -1.0000         0.0         0.0
         0.0         0.0         0.0         0.0         0.0     -1.0000      1.0000
         0.0         0.0         0.0         0.0         0.0         0.0     -1.0000

***MATRIX B***
     -1.0000         0.0         0.0         0.0         0.0         0.0         0.0
      1.0000     -1.0000         0.0         0.0         0.0         0.0         0.0
         0.0      1.0000     -1.0000         0.0         0.0         0.0         0.0
         0.0         0.0      0.5000     -1.0000         0.0         0.0         0.0
         0.0         0.0         0.0      1.0000     -1.0000         0.0         0.0
         0.0         0.0      0.5000         0.0         0.0     -1.0000         0.0
         0.0         0.0         0.0         0.0         0.0      1.0000     -1.0000

***FEED MATRIX***
         0.0         0.0         0.0
         0.0         0.0         0.0
         0.0         0.0         0.0
     40.0000     20.0000     20.0000
         0.0         0.0         0.0
         0.0         0.0         0.0
         0.0         0.0         0.0

***VAPOR FLOW VECTOR***
     40.0000    160.0000    120.0000    120.0000     40.0000     40.0000     40.0000

***LIQUID FLOW VECTOR***
    120.0000    120.0000    120.0000     60.0000     20.0000     60.0000     20.0000
```

```
*****RESULTS FOR ITERATION   1 BEGIN HERE*****

**ASSUMED TEMPERATURE VECTOR**
     39.0000      42.0000      45.0000      48.0000      51.0000      46.0000      48.0000

**LIQUID COMPOSITION MATRIX**
      0.6260       0.2585       0.1541
      0.5792       0.3004       0.2320
      0.5133       0.3057       0.2890
      0.4238       0.2874       0.3468
      0.3431       0.2823       0.4126
      0.4744       0.3238       0.3372
      0.4050       0.3354       0.4218

**VAPOR COMPOSITION MATRIX**
      0.6259       0.1911       0.0828
      0.6260       0.2417       0.1363
      0.5987       0.2672       0.1854
      0.5328       0.2725       0.2424
      0.4642       0.2899       0.3139
      0.5674       0.2908       0.2226
      0.5091       0.3180       0.2949

**MATERIAL BALANCE ERROR VECTOR IS**
      0.1387       0.1077       0.0568       0.0103      -0.0299       0.0546       0.0403

**MATERIAL BALANCE ERROR NORM IS    0.19915E 00**

**CORRECTED TEMPERATURE VECTOR**
     44.7101      46.0128      47.0447      48.3775      49.9178      47.9130      49.3645
```

```
*****RESULTS FOR ITERATION   2 BEGIN HERE*****

**ASSUMED TEMPERATURE VECTOR**
    44.7101     46.0128     47.0447     48.3775     49.9178     47.9130     49.3645

**LIQUID COMPOSITION MATRIX**
     0.5763      0.2533      0.1640
     0.5007      0.2726      0.2257
     0.4511      0.2767      0.2752
     0.3974      0.2712      0.3349
     0.3279      0.2716      0.4057
     0.4049      0.2859      0.3154
     0.3375      0.2891      0.3856

**VAPOR COMPOSITION MATRIX**
     0.6673      0.2196      0.1043
     0.5990      0.2449      0.1491
     0.5538      0.2556      0.1872
     0.5042      0.2597      0.2366
     0.4321      0.2710      0.2994
     0.5079      0.2704      0.2199
     0.4387      0.2843      0.2802

**MATERIAL BALANCE ERROR VECTOR IS**
     0.0024      0.0060      0.0063      0.0029      0.0027      0.0079      0.0090

**MATERIAL BALANCE ERROR NORM IS    0.15546E-01**

**CORRECTED TEMPERATURE VECTOR**
    44.8013     46.2430     47.2879     48.4883     50.0206     48.2175     49.7092
```

```
*****RESULTS FOR ITERATION   3 BEGIN HERE*****

**ASSUMED TEMPERATURE VECTOR**
     44.8013      46.2430      47.2879      48.4883      50.0206      48.2175      49.7092

**LIQUID COMPOSITION MATRIX**
      0.5781       0.2553       0.1663
      0.4997       0.2732       0.2274
      0.4498       0.2761       0.2757
      0.3957       0.2703       0.3345
      0.3259       0.2702       0.4045
      0.4012       0.2844       0.3153
      0.3323       0.2859       0.3834

**VAPOR COMPOSITION MATRIX**
      0.6709       0.2219       0.1060
      0.6013       0.2470       0.1512
      0.5543       0.2568       0.1888
      0.5034       0.2597       0.2371
      0.4305       0.2704       0.2994
      0.5070       0.2712       0.2218
      0.4356       0.2837       0.2813

**MATERIAL BALANCE ERROR VECTOR IS**
      0.0008       0.0008       0.0006       0.0003       0.0003       0.0009       0.0009

**MATERIAL BALANCE ERROR NORM IS    0.19088E-02**

******CALCULATION TERMINATED******
******ERROR NORM LESS THAN 0.01******
```

I. PROBLEM IDENTIFICATION

1. Title: Amundsen-Pontinen Distillation
2. Author: Leonard L. Hovey
3. Affiliation: University of Wyoming

II. TECHNICAL DESCRIPTION

1. Problem Statement:

A cresylic acid fractionation plant has a feed with the following composition:

Phenol	12.0 mol. %
o-cresol	14.0 " "
"compound A"	1.0 " "
m-cresol	21.0 " "
p-cresol	9.0 " "
o-ethyl phenol	3.0 " "
2-4 & 2-5 xylenols	14.0 " "
2-3 xylenol	6.0 " "
3-4 xylenol	4.0 " "
3-5 xylenol	11.0 " "
heavier components	5.0 " "

This material will be fractionated in a column with 48 theoretical trays, a partial reboiler and a total condenser. The feed is introduced above the 21st theoretical tray (below 27th theoretical tray from the top). The tower overhead pressure is 100 mm Hg absolute. It is estimated that the pressure drop per tray will be 7.0 mm Hg. It is desired to produce a phenol, o-cresol fraction overhead with less than 2.0% material heavier than o-cresol while producing a bottom fraction with less than 0.3% phenol and o-cresol. Preparatory to making an economic evaluation of the column operation you are requested to determine:

1. reflux ratio
2. condenser duty
3. reboiler duty
4. overhead temperature

5. overhead composition
6. bottom temperature
7. bottoms composition

The feed withdrawn as overhead product is 26%. The recommended initial reflux ratio is 5 to 1.

The following assumptions may be reasonably made for this solution.

1. Heat losses from the equipment are negligible.
2. The specific heat and latent heat of each component is constant over the temperature and pressure range of the equipment.
3. Raoult's law is applicable.

Use the Pontinen-Amundson method(1) with a tridiagonal matrix solution technique.(2)

The following liquid heat capacities and heats of vaporization may be used. (Heat of vaporization estimated with the Nerst-Bingham rule. Liquid heat capacity based on average heat capacity of 0.526 BTU/LB°F).

Component	λ_v BTU/LB Mole	C_{P_L} BTU/LB Mole °F
Phenol	18027.	49.5
o-cresol	18461.	56.9
compound A	18830.	64.3
m-cresol	19051.	56.9
p-cresol	19003.	56.9
o-ethyl phenol	19285.	64.3
2-4 & 2-5 xylenol	19483.	64.3
2-3 xylenol	19807.	64.3
3-4 xylenol	20169.	64.3
3-5 xylenol	19883.	64.3
heavier components	20664.	71.7

The vapor pressures have been fit to the following equation (least square fit to data in Perry's Handbook)

$$Ln\ (P) = A + B(\frac{1}{T}) + C(\frac{1}{T})^2$$

---

(1) Buford D. Smith, "Design of Equilibrium Stage Processes" McGraw-Hill Book Company, Ind., New York, 1963.

(2) Brice Carnahan, H. A. Luther, and James O. Wilkes, "Applied Numerical Methods" John Wiley & Sons, Inc., New York, 1969.

where P is mm Hg.

T is °K.

Compound	A	B	C
Phenol	14.5501	-1555.47	-931,947.
o-cresol	16.6206	-3452.84	-547,637.
compound A	16.7449	-3905.90	-404,178.
m-cresol	14.0956	-1297.77	-1,071,880.
p-cresol	16.8285	-3475.84	-647,160.
o-ethyl phenol	18.5543	-5375.14	-170,757.
2-4 & 2-5 xylenols	12.4528	- 12.73	-1,353,720.
2-3 xylenol	20.0222	-6639.81	+ 29,882.
3-4 xylenol	19.1813	-5734.60	-261,170.
3-5 xylenol	20.1931	-6564.93	- 57,485.
heavier components	18.9286	-5730.00	-261,200.

2. Problem Formulation and Technical Analysis: (Reference Chapter 10, section 6 of "Design of Equilibrium Stage Processes" by Buford D. Smith, 1963).

A. Material Balance:

A mass balance for any component i can be made around each stage n as follows:

stage 1 (reboiler) (n=1)

$$-(B + V_n K_{ni}) X_{ni} + (V_n + B) X_{(n+1)i} = 0 \qquad (1)$$

Stripping section (n = 2 to M)

$$(V_{(n-1)} K_{(n-1)i}) X_{(n-1)i} - (V_{(n-1)} + B + V_n K_{ni}) X_{ni} + (V_n + B) X_{(n+1)i} = 0 \qquad (2)$$

Feed stage n = M + 1

$$(V_{(n-1)} K_{(n-1)i}) X_{(n-1)i} - (V_{(n-1)} + B + V_n K_{ni}) X_{ni} + (V_n - D) X_{(n+1)i} = -F X_{Fi} \qquad (3)$$

Rectifying section (n = M + 2 to N)

$$(V_{(n-1)} K_{(n-1)i}) X_{(n-1)i} - (V_{(n-1)} - D + V_n K_{ni}) X_{ni} + (V_n - D) X_{(n+1)i} = 0 \qquad (4)$$

Total condenser $(n = N + 1)$

$$(V_{(n-1)}K_{(n-1)i})X_{(n-1)i} - (V_n)X_{ni} = 0 \tag{5}$$

This can be expressed as the tridiagonal matrix $\bar{\bar{M}}$ times the single-column matrix $\bar{X}$ equals the single-column matrix $\bar{F}$ for each component i. $\bar{M}_i\bar{X}_i = \bar{F}_i$

3. Solution of Matrix Equation:

The tridiagonal matrix $\bar{M}$ is expressed as a $(N+1)$ by 4 matrix where the fourth column is the single-column matrix $\bar{F}$. The first column is the coefficient of the $x_{(n-1)i}$ term. The second column is the coefficient of the x_{ni} term. The third column is the coefficient of the $x_{(n+1)i}$ term.

The subroutine TOMSOL is now called to solve the matrix equation and returns the value of x_{ni} in column one of our $(N+1)$ by 4 matrix. (Reference pp 441-2, "Applied Numerical Methods" by Brice Carnahan, H. A. Luther, and J. O. Wilkes, 1969). In the following A_i refers to the first column, B_i refers to the second column, C_i refers to the third column, and D_i refers to the fourth column of the $(N+1)$ by 4 matrix.

$$\beta_1 = B_1 \tag{6}$$

$$\gamma_1 = D_1/\beta_1 \tag{7}$$

$$Q_1 = C_1/\beta_1 \tag{8}$$

$$\beta_i = B_i - A_iQ_{(i-1)} \qquad i = 2 \text{ to } N + 1 \tag{9}$$

$$Q_i = C_i/\beta_i \qquad i = 2 \text{ to } N + 1 \tag{10}$$

$$\gamma_i = D_i - \frac{A_i\gamma_{(i-1)}}{\beta_i} \qquad i = 2 \text{ to } N + 1 \tag{11}$$

$$x_i = \gamma_i \text{ for } i = N + 1 \tag{12}$$

$$x_i = \gamma_i - Q_i\, X_{(i+1)} \text{ for } i = N \text{ to } 1 \tag{13}$$

Since negative mole fractions are not physically possible, any negative values of mole fraction are set equal to zero. The mole fractions on each tray are summed and checked to see if they are within the convergence error limit of 1.000. If not, a new temperature profile will be assumed. The mole fractions on each tray are then normalized to give a summation of 1.000 before calculating the new temperature profile.

C. Temperature Profile:

The initial temperature profile is taken as constant at the feed temperature. A Newton approximation is used to adjust each tray to its bubble point for subsequent iterations. A maximum adjustment of 100°F on any temperature per iteration has been used to avoid wild adjustments which lead to non-convergence.

$$\phi_n = \sum_{i=1}^{NC} K_{ni} X_{ni} \tag{14}$$

Letting T'_n be the last temperature and T_n the adjusted temperature,

$$\phi_n(T_n) = \phi_n(T'_n) + (T_n - T'_n) \frac{\partial \phi_n}{\partial T_n} \tag{15}$$

Since at the correct temperature $\phi_n = 1$,

$$T_n = T'_n + \frac{(1 - \phi_n(T'_n))}{(\frac{\partial \phi_n}{\partial T_n})} \tag{16}$$

$$\frac{\partial \phi_n}{\partial T_n} = \sum_{i=1}^{NC} X_{ni} \frac{\partial K_{ni}}{(\partial T_n)} \tag{17}$$

K values and $\frac{\partial K}{\partial T}$ values are calculated in the subroutine EK. Raoults law is assumed and vapor pressure data of the form

$$\text{Ln}(P) = A + \frac{B}{T} + \frac{CC}{T^2} \tag{18}$$

where P is in mm Hg

T is in °K

are used in this subroutine.

D. Vapor Profile:

The initial vapor profile is taken as constant throughout the tower at the value of the specified vapor going to the condenser. The adjusted vapor profile is adjusted on the basis of an energy balance using the adjusted compositions and temperatures. Vapor profile adjustment is not started until temperature profile adjustments are less than 20°F.

Molar stream enthalpies relative to liquid at 0°F are calculated assuming ideal solutions.

$$H_{vn} = \sum_{i=1}^{NC} Y_{ni} H_{vni} = \sum_{i=1}^{NC} K_{ni} X_{ni} H_{vni} \tag{19}$$

$$h_{Ln} = \sum_{i=1}^{NC} X_{ni} h_{Lni} \tag{20}$$

Liquid enthalpy has been taken as

$$h_{Lni} = X_{ni} (C_{P_L})_i T_n \tag{21}$$

and vapor enthalpy as

$$H_{vni} = Y_{ni} (h_{Lni} + \lambda_{vi}) \tag{22}$$

$$H_{vni} = K_{ni} X_{ni} (h_{Lni} + \lambda_{vi}) \tag{23}$$

Since V_N the vapor to the overhead condenser is fixed, the condenser duty is,

$$Q_c = V_N (H_{VN} - h_{L(N+1)}) \tag{24}$$

An overall heat balance around the column gives the reboiler duty

$$Q_R = D\, h_{L(N+1)} + B\, h_{L1} + Q_c - FH_F \tag{25}$$

An energy balance now on each stage gives the moles of vapor from the stage.

Reboiler (n = 1)

$$V_n = \frac{B(h_{Ln} - h_{L(n+1)}) - Q_R}{(h_{L(n+1)} - H_{vn})} \tag{26}$$

Stages below the feed (n = 2 to M)

$$V_n = \frac{B(h_{Ln} - h_{L(n+1)}) - V_{(n-1)}(H_{v(n-1)} - h_{Ln})}{(h_{L(n+1)} - H_{vn})} \tag{27}$$

Feed stage (n = M + 1)

$$V_n = \frac{D\ h_{L(n+1)} + B\ h_{Ln} - F\ H_F - V_{(n-1)}(H_{v(n-1)} - h_{Ln})}{(h_{L(n+1)} - H_{vn})} \tag{28}$$

Above the feed stage (n = M + 2 to N)

$$V_n = \frac{D(h_{L(n+1)} - h_{Ln}) - V_{(n-1)}(H_{v(n-1)} - h_{Ln})}{(h_{L(n+1)} - H_{vn})} \tag{29}$$

3. Method of Solution:

The pressure on each tray is calculated by adding the pressure drop per tray times the number of trays from the top to the top pressure. The initial vapor profile is assumed as the vapor to the condenser and the initial temperature profile is assumed as the feed temperature.

The mass balance equations are solved for the composition of each tray. The composition of all the trays is checked against the convergence error limit. If convergence has not been reached a new temperature profile is calculated based on the bubble point of the tray composition calculated. A new vapor profile is calculated on the basis of the energy balance.

4. References and Data: The reference texts are listed in the "Problem Formulation and Technical Analysis" section. Data can be taken from the standard reference texts such as Perry's Handbook.

5. Solution:

A. Input required

The program requires input of the following data:

1. Number of total theoretical stages"N" (must be in the range 1 to 49)

2. Number of theoretical stages below the feed stage "M" (must be in the range 2 to 47)

3. Number of components "NC" (must be in the range 1 to 12)

4. Feed mole fraction of each component "Z"

5. Volatility data, "A", "B", "CC" for each component in the form $\text{Ln}(P) = A + \frac{B}{T} + \frac{CC}{T^2}$ where P is mm Hg
T is °K

6. Enthalpy data for each component. Heat of vaporization "CHV" is BTU/Lb Mole and liquid heat capacity "CPL" in BTU/(Lb Mole °F)

7. Overhead product rate per 100 moles of feed "TOP"

8. Bottoms product rate per 100 moles of feed "BOTT"

9. Temperature of the feed in °F "TFEED"

10. Enthalpy of the feed per mole referenced to liquid at 0°F "HFEED"

11. Moles vapor to the overhead condenser per 100 moles of feed "VINIT"

12. Pressure drop per tray in mm Hg "PDPTR"

Plus the following optional values.

13. Top pressure in mm Hg "TOPP"; this is assigned the value 760 if unspecified.

14. The convergence error limit as mole fraction "ERROR"; this is assigned a value of 0.01 if unspecified.

15. The maximum number of iterations "CYCLE"; this is assigned a value of 20 if unspecified.

16. An index to give output of all the trays where only overhead and bottoms aren't enough "NIND"; if NIND = 0 only top and bottom are written.

17. An index for making another run "INDEX." If INDEX = 1 you will recycle to the third portion of the data. If INDEX = 2 you will recycle to the second portion of the data. If INDEX = 3 you will recycle to the first portion of the data.

Data Input

first portion - 1 card
FORMAT (3I3, 3F10.5, 2I3)
Items: N, M, NC, TOPP, PDPTR, ERROR, CYCLE, NIND
second portion - NC cards
FORMAT (6F10.5)

Items: Z, A, B, CC, CHV, CPL

third portion - 1 card

FORMAT (I2, 5F10.5)

Items: INDEX, TOP, BOTT, TFEED, HFEED, VINIT

B. Results:

The output gives the top and bottoms composition by component number as X(I). The vapor composition in equilibrium with the liquid products is also given. The temperature of overheads and bottoms is given. The heat load on the condenser and reboiler as well as the overhead, bottom and reflux rates are given per 100 moles of feed.

Individual tray composition, pressure, temperature and flows can also be obtained by setting NIND = 1 on the first data card.

C. Discussion of the Results:

Most problems of up to the maximum size will require about 15-25 iterations for an error limit of 0.01 on convergence. If convergence has not been obtained this will be indicated. Even for an unconverged run the overhead and bottoms temperatures and compositions are surprisingly good. You can also get the sum of mole fractions on the trays which are not within the convergence limit.

III. EDUCATIONAL (PEDOGOLOGICAL) ASPECTS:

1. Description of Past Usage: I have used this problem, or a variation of it, in my senior level stagewise operations course and in my senior level plant design course.

2. Concepts Demonstrated:

   a) Development of mass and energy balances incorporating the equilibrium relationship to obtain the solution to a distillation separation

   b) Preliminary assumptions required for solution of a distillation problem using the Amundsen-Pontinen method.

   c) Incorporation of the convergence limit.

   d) Use of a tridiagonal matrix solution technique.

   e) Use of computer to solve a complex distillation separation problem.

3. Evaluation of Usage:

This was originally given as a month assignment to write the program and solve the problem in the stagewise operations class. It was subsequently modified to be used in the plant design class for the final calculations of the problem "Production of Psudocumene-Preliminary Design and Economic Study" by R. J. Hengstebeck and J. T. Banchero.

4. Nature of Assignment: The student will determine if a design arrived at by one of the short cut distillation methods will give the desired operation.

V. PROGRAM DESCRIPTION

This program calculates the overhead and bottoms compositions of a distillation column using the Amundsen-Pontinen method. It uses a subroutine, EK(N,NC), to calculate the K values and another subroutine, TOMSOL (N+1), to solve the tridiagonal matrix material balance equations. All input and output is via the main program.

The program is limited to multicomponent distillations of 12 components or less and 49 stages or less. These limitations are becuase of dimension sizes of the variables and could be expanded. The calculations are based on 100 moles of feed.

The program was developed on the XDS Sigma 7 using timesharing. It has been run on the Sigma 7 under both batch and timesharing.

The program has been used for several large distillation problems in the manner presented and also in modified versions. An expanded version of the program to take 16 components and 129 stages with a different form of vapor pressure equation has been used in the distillation tower design of the design problem by R. J. Hengstebeck and J. T. Banchero.

Argument List and Program Variables:

A, the quantity in the vapor pressure equation $Ln(P) = A + B/T + CC/T^2$. This is an array of 12 real numbers and is both an input and and output.

ABS, the absolute value subroutine.

B, the quantity in the vapor pressure equation $Ln(P) = A + B/T + CC/T^2$. This is an array of 12 real numbers and is both an input and an output.

BOTT, the moles of bottoms per 100 moles of feed. This is represented by B in the development by Smith. This is a real scalar quantity and is both an input and output.

CC, the quantity in the vapor pressure equation $Ln(P) = A + B/T + CC/T^2$. This is an array of 12 real numbers and is both an input and an output.

CHV, the average molar heat of vaporization in BTU per pound mole. This is an array of 12 real numbers and is both an input and an output.

COEFF, the matrix of the coefficients of the three diagonals in the mass balance equations and the right hand side of the equations. This is a matrix of 50 rows and 4 columns of real numbers. It is neither an input nor output.

CPL, the average molar heat capacity of the liquid in BTU per pound mole per degree fahrenheit. This is an array of 12 real numbers and is both an input and an output.

CYCLE, the maximum number of iteration cycles. This is an integer scalar quantity. It is an input but will be assigned the value of 20 if no input value is given.

DENOM, a dummy variable calculated in the program. This is a real scalar quantity. It is neither an input nor output.

DIFK, the partial differential of K_i with respect to temperature. This is a real matrix of N + 1 by NC values. It is neither an input nor output.

DIFPHI, the summation of the product of mole fraction times DIFK on each stage. This is an array of (N+1) real numbers. It is neither an input nor output.

EK, the external subroutine supplied with the main program for calculating the K values and DIFK values. It contains no input nor output. The argument list is (N,NC) the number of stages and the number of components.

ERROR, the mole fraction tolerance or error in composition which will be allowed on any tray. This is a real scalar quantity. It is an input and an output but will be assigned a value of 0.01 if it is not given in the data input.

FEED, the moles per hour of feed, This is specified as 100 in the program. This is a real scalar quantity. It is neither an input nor output.

HFEED, the enthalpy of the feed in BTU's/(Lb Mole) with reference to liquid at 0°F. This is a real scalar quantity. It is an input value.

HLIQ, the enthalpy of the liquid on a stage in BTU/Lb Mole. This is an array of N real numbers. It is neither an input nor output.

HVAP, the enthalpy of the vapor on a stage in BTU/Lb Mole. This is an array of N real numbers. It is neither an input nor output.

I, II, IM1, IP1, dummy integer variables used in do loops.

IIN, the unit number of the device for data input. This is an integer scalar quantity. It is assigned a value of 5 in the program with a data statement.

INDEX, an index to indicate if more runs are desired. This is an integer scalar quantity. It is an input.

IOUT, the unit number of the output device on which error messages will appear. This is an integer scalar quantity. It is assigned a value of 6 in the program with a data statement.

IOUT1, the unit number of the output device on which the main program output will appear. This is an integer scalar quantity. It is assigned a value of 7 in the program with a data statement.

IOUT2, the unit number of the output device on which the unadjusted mole fraction for unconverged stages will appear. This is an integer scalar quantity. It is assigned a value of 8 in the program with a data statement.

IOUT3, the unit number of the output device on which the individual tray results will appear if NIND $\neq$ 0. This is an integer scalar quantity. It is assigned a value of 9 in the program with a data statement.

J, K, L, dummy integer variables used in do loops.

LIQ, the moles of liquid leaving any stage. This is an array of (N+1) real numbers. It is an output.

M, the number of theoretical stages below the feed. This is an integer scalar quantity. It is both an input and an output.

MM, the number of the feed stage (M+1). This is an integer scalar quantity. It is computed internally and is neither an input nor output.

MMM, the number of the stage above the feed stage (M+2). This is an integer scalar quantity. It is computed internally and is neither an input nor output.

N, the total number of total theoretical stages in the column. This is an integer scalar quantity. It is an input and output.

NBILL, the number of the present iteration. This is an integer scalar variable. It is an output.

NC, the number of components. This is an integer scalar quantity. It is an input.

NCONV, an indicator which is assigned a value of 1 if convergence was not obtained. This is an integer scalar quantity. It is neither an input nor output.

NFLAG, an indicator which is assigned a value of 1 if a new run is being made with approximately the same temperature profile as the previous run (when INDEX = 1). This is an integer scalar quantity. It is neither an input nor output.

NIND, an indicator which is given a non zero value if each individual stage result is desired. This is an integer scalar quantity. It is an input.

NM, NM1, dummy integer variables used in do loops.

NMTWO, a dummy variable calculated in the program. This is a real scalar quantity. It is neither an input nor output.

NN, the overhead condenser stage, (N+1). This is an integer scalar quantity. It is neither an input nor output.

NONE, a dummy variable calculated in the program. This is a real scalar quantity. It is neither an input nor output.

NPOINT, an indicator which is assigned a value of 2 if a stage sum of mole fraction differs from 1.00 by more than the convergence error. This is an integer scalar quantity. It is neither an input nor output.

NRUN, the number of the case being calculated. This is an integer scalar quantity. It is an output.

PDPTR, the pressure drop per tray. This is a real scalar quantity. It is an input.

PHI, the summation of K times mole fraction (or vapor mole fraction) on any stage. This is a real scalar quantity. It is neither an input nor output.

QC, the energy removed by the condenser in BTU's per 100 moles of feed. This is a real scalar quantity. It is an output.

QR, the energy supplied to the reboiler in BTU's per 100 moles of feed. This is a real scalar quantity. It is an output.

REFLUX, the moles of reflux returned to the column per 100 moles of feed. This is a real scalar quantity. It is an output.

SOME, a dummy variable assigned the value of the final unadjusted mole fraction on a tray. This is a real scalar quantity. It is neither an input nor output.

SUM, the sum of the unadjusted mole fraction on a tray, which is used to get the adjusted mole fraction on the tray. This is a real scalar quantity. It is neither an input nor output.

TADJ, a dummy variable used in adjusting the temperature profile. This is a real scalar quantity. It is neither an input nor output.

TADJA, a dummy variable used as an indicator that vapor profile should not be adjusted until the temperature profile is closer. This is a real scalar quantity. It is neither an input nor output.

TEMP, the temperature, in °F, of a stage. This is a real array. It is an output.

TFEED, the temperature of the feed in °F. This is a real scalar quantity. It is an input and output.

TN, the real number which is a function of the do loop index. This is a real scalar quantity. It is neither an input nor output.

TOMSOL, the external subroutine supplied with the main program for solving the tridiagonal matrix. It contains no input nor output. The argument list is (N+1), the number of unknowns.

TOP, the number of moles of overhead product per 100 moles of feed. This is a real scalar quantity. It is both an input and output.

TOPP, the top of the tower pressure in mm Hg. This is a real scalar quantity. It is an input but will be assigned the value of 760 if no input value is given.

TRAY, the sum of the liquid mole fraction on any tray. This is an array of real numbers. It may be an output.

V, the moles of vapor leaving any stage. This is an array of real numbers. It is an output.

VINIT, the moles of vapor from the Nth tray to the overhead condenser.

This is a real scalar quantity. It is an input.

X, the liquid mole fraction of a component on a tray. This is a matrix of real numbers. It is an output.

YY, the vapor mole fraction of a given component on a given tray. This is a real scalar quantity. It is an output.

Z, the mole fraction of a component in the feed. This is an array of real numbers. It is an input and output.

Data Input:

The program requires input of the following data:

1. Number of total stages theoretical - "N" (must be in the range 1 to 49)
2. Number of theoretical stages below the feed stage - "M" (must be in the range 2 to 47)
3. Number of components - "NC" (must be in the range 1 to 12)
4. Feed mole fraction of each component - "Z"
5. Volatility data, "A", "B", "CC" for each component in the form $Ln(P) = A + B/T + CC/T^2$ where P is mm Hg
   T is °K
6. Enthalpy data for each component. Average heat of vaporization "CHV" in BTU/Lb Mole and average liquid heat capacity "CPL" in BTU/(Lb Mole °F)
7. Overhead product rate per 100 moles of feed "TOP"
8. Bottoms product rate per 100 moles of feed "BOTT"
9. Temperature of the feed in °F "TFEED"
10. Enthalpy of the feed per mole referenced to liquid at 0°F "HFEED"
11. Moles vapor to the overhead condenser per 100 moles of feed "VINIT"
12. Pressure drop per tray in mm Hg "PDPTR"

Plus the following optional values.

13. Top pressure in mm Hg "TOPP" this is assigned the value 760 if unspecified.
14. The convergence error limit as mole fraction "ERROR" this is assigned a value of 0.01 if unspecified.

15. The maximum number of iterations "CYCLE" this is assigned a value of 20 if unspecified
16. An index to give output of all the trays where only overhead and bottoms aren't enough "NIND", if NIND = 0 only top and bottom are written.
17. An index for making another run "INDEX." If INDEX = 1 you will recycle to the third portion of the data. If INDEX = 2 you will recycle to the second portion of the data. If INDEX = 3 you will recycle to the first portion of the data.

Data Input

first portion - 1 card
FORMAT (3I3, 3F10.5, 2I3)
Items: N, M, NC, TOPP, PDPTR, ERROR, CYCLE, NIND

second portion - NC cards
FORMAT (6F10.5)
Items: Z, A, B, CC, CHV, CPL

third portion - 1 card
FORMAT (I2, 5F10.5)
Items: INDEX, TOP, BOTT, TFEED, HFEED, VINIT

Output:

The output of the program are self explanatory. Tray 1 is the bottoms product and tray (N+1) is the overhead product. X values are the liquid mole fractions. Examples are attached. Table 1 is a listing of the input data on feed composition, volatility and enthalpy constants. Table 2 is a listing of the normal output. Tray 1 is the reboiler. Tray N+1, (50), is the overhead condenser. Table 3 is the first page of the listing for the case NIND = 1. This was made with IOUT, IOUT1, IOUT2, and IOUT3 all assigned as the line printer. Table 4 is the first page of the listing for an unconverged run. This is also with all output units assigned to the line printer.

The three diagnostics are FORMAT statements 117, 118, and 119. These are self explanatory namely that the total number of trays, N, the number of trays below the feed, M, or the number of components, NC is outside the permissible range of the program.

Table 1

```
INPUT DATA

COMP FEED MOLE   LN (P) = A + B/T + CC/(T*T)   HEAT OF      LIQ HEAT

     FRACTION        A          B         CC   VAPORIZATION  CAPACITY


 1    .12000    14.5501  -1555.47   -931947.    18027.00      49.50
 2    .14000    16.6206  -3452.84   -547637.    18461.00      56.90
 3    .01000    16.7449  -3905.90   -404178.    18830.00      64.30
 4    .21000    14.0956  -1297.77 -1071880.     19051.00      56.90
 5    .09000    16.8285  -3475.84   -647160.    19003.00      56.90
 6    .03000    18.5543  -5375.14   -170757.    19285.00      64.30
 7    .14000    12.4528    -12.73 -1353720.     19483.00      64.30
 8    .06000    20.0222  -6639.81     29882.    19807.00      64.30
 9    .04000    19.1813  -5734.60   -261170.    20169.00      64.30
10    .11000    20.1931  -6564.93    -57485.    19883.00      64.30
11    .05000    18.9286  -5730.00   -261200.    20664.00      71.70
```

Table 2

```
RUN  1  WITH 49  TCTAL TRAYS AND 21 BELOW THE FEED TRAY.

CONVERGENCE ERROR LIMIT IS   .01000 AND THE FEED TEMP. IS  100.00 DEGREES F

FINAL SOLUTION REQUIREC  14  ITERATIONS

TRAY   MM PRESS   TEMP  F   MOLS VAPOR  LIQUID MOLS
  1     443.0     374.35     221.01     74.00
                 X( 1) =  .000052          Y( 1) =  .000111
                 X( 2) =  .011212          Y( 2) =  .019033
                 X( 3) =  .007098          Y( 3) =  .010009
                 X( 4) =  .279763          Y( 4) =  .346362
                 X( 5) =  .121014          Y( 5) =  .151443
                 X( 6) =  .040517          Y( 6) =  .043451
                 X( 7) =  .189114          Y( 7) =  .195125
                 X( 8) =  .081053          Y( 8) =  .062701
                 X( 9) =  .054036          Y( 9) =  .032794
                 X(10) =  .148598          Y(10) =  .106733
                 X(11) =  .067545          Y(11) =  .032152

TRAY   MM PRESS   TEMP  F   MOLS VAPOR  LIQUID MOLS
 50     100.0     255.87        .00    130.00
                 X( 1) =  .461814          Y( 1) =  .532184
                 X( 2) =  .507025          Y( 2) =  .445784
                 X( 3) =  .018272          Y( 3) =  .014422
                 X( 4) =  .011209          Y( 4) =  .006471
                 X( 5) =  .001611          Y( 5) =  .000877
                 X( 6) =  .000028          Y( 6) =  .000015
                 X( 7) =  .000041          Y( 7) =  .000019
                 X( 8) =  .000000          Y( 8) =  .000000
                 X( 9) =  .000000          Y( 9) =  .000000
                 X(10) =  .000000          Y(10) =  .000000
                 X(11) =  .000000          Y(11) =  .000000

QC =  .288269E 07  QR =  .435359E 07  BOTTOMS ARE 74.000000

DISTILLATE IS 26.000000  REFLUX IS 130.000000
```

Table 3

```
  RUN   1  WITH 49  TOTAL TRAYS AND 21 BELOW THE FEED TRAY.

CONVERGENCE ERROR LIMIT IS   .01000 AND THE FEED TEMP. IS  100.00 DEGREES F

 FINAL SOLUTION REQUIRED   8  ITERATIONS

  TRAY   MM PRESS   TEMP  F   MOLS VAPOR   LIQUID MOLS
   1      443.0     374.58     289.50      74.00
                  X( 1) =   .000011          Y( 1) =   .000024
                  X( 2) =   .004092          Y( 2) =   .006970
                  X( 3) =   .009094          Y( 3) =   .012868
                  X( 4) =   .283759          Y( 4) =   .352530
                  X( 5) =   .121657          Y( 5) =   .152807
                  X( 6) =   .040560          Y( 6) =   .043653
                  X( 7) =   .189285          Y( 7) =   .195973
                  X( 8) =   .081125          Y( 8) =   .062996
                  X( 9) =   .054083          Y( 9) =   .032956
                  X(10) =   .148730          Y(10) =   .107255
                  X(11) =   .067604          Y(11) =   .032311

  TRAY   MM PRESS   TEMP  F   MOLS VAPOR   LIQUID MOLS
   2      436.0     370.13     290.49     363.50
                  X( 1) =   .000021          Y( 1) =   .000043
                  X( 2) =   .006382          Y( 2) =   .010326
                  X( 3) =   .012096          Y( 3) =   .016288
                  X( 4) =   .338437          Y( 4) =   .398849
                  X( 5) =   .146426          Y( 5) =   .173778
                  X( 6) =   .043012          Y( 6) =   .043820
                  X( 7) =   .194559          Y( 7) =   .191226
                  X( 8) =   .066669          Y( 8) =   .048783
                  X( 9) =   .037247          Y( 9) =   .021299
                  X(10) =   .115667          Y(10) =   .078322
                  X(11) =   .039485          Y(11) =   .017710

  TRAY   MM PRESS   TEMP  F   MOLS VAPOR   LIQUID MOLS
   3      429.0     367.07     291.02     364.49
                  X( 1) =   .000037          Y( 1) =   .000073
                  X( 2) =   .009058          Y( 2) =   .014214
                  X( 3) =   .014823          Y( 3) =   .019387
                  X( 4) =   .375355          Y( 4) =   .428640
                  X( 5) =   .163141          Y( 5) =   .187112
                  X( 6) =   .043143          Y( 6) =   .042537
                  X( 7) =   .190764          Y( 7) =   .181771
                  X( 8) =   .055328          Y( 8) =   .039055
                  X( 9) =   .027944          Y( 9) =   .015371
                  X(10) =   .092581          Y(10) =   .060329
                  X(11) =   .027828          Y(11) =   .012007

  TRAY   MM PRESS   TEMP  F   MOLS VAPOR   LIQUID MOLS
   4      422.0     364.83     291.13     365.02
                  X( 1) =   .000061          Y( 1) =   .000119
                  X( 2) =   .012158          Y( 2) =   .018738
                  X( 3) =   .017294          Y( 3) =   .022236
```

Table 4

```
   RUN  1  WITH 49  TOTAL TRAYS AND 21 BELOW THE FEED TRAY.

CONVERGENCE ERROR LIMIT IS   .01000 AND THE FEED TEMP. IS  100.00 DEGREES F

 FINAL SOLUTION REQUIRED   7  ITERATIONS

   THIS DOES NOT REPRESENT A CONVERGED SOLUTION
 TRAY    7  SUM OF X  IS     .989707
 TRAY    8  SUM OF X  IS     .986343
 TRAY    9  SUM OF X  IS     .982647
 TRAY   10  SUM OF X  IS     .978843
 TRAY   11  SUM OF X  IS     .975103
 TRAY   12  SUM OF X  IS     .971563
 TRAY   13  SUM OF X  IS     .968354
 TRAY   14  SUM OF X  IS     .965579
 TRAY   15  SUM OF X  IS     .963387
 TRAY   16  SUM OF X  IS     .961948
 TRAY   17  SUM OF X  IS     .961459
 TRAY   18  SUM OF X  IS     .962177
 TRAY   19  SUM OF X  IS     .964432
 TRAY   20  SUM OF X  IS     .968632
 TRAY   21  SUM OF X  IS     .975348
 TRAY   22  SUM OF X  IS     .985351
 TRAY   25  SUM OF X  IS    1.015544
 TRAY   26  SUM OF X  IS    1.020376
 TRAY   27  SUM OF X  IS    1.023649
 TRAY   28  SUM OF X  IS    1.025610
 TRAY   29  SUM OF X  IS    1.026525
 TRAY   30  SUM OF X  IS    1.026692
 TRAY   31  SUM OF X  IS    1.026366
 TRAY   32  SUM OF X  IS    1.025745
 TRAY   33  SUM OF X  IS    1.024954
 TRAY   34  SUM OF X  IS    1.024069
 TRAY   35  SUM OF X  IS    1.023133
 TRAY   36  SUM OF X  IS    1.022154
 TRAY   37  SUM OF X  IS    1.021113
 TRAY   38  SUM OF X  IS    1.020000
 TRAY   39  SUM OF X  IS    1.018794
 TRAY   40  SUM OF X  IS    1.017473
 TRAY   41  SUM OF X  IS    1.016039
 TRAY   42  SUM OF X  IS    1.014505
 TRAY   43  SUM OF X  IS    1.012891
 TRAY   44  SUM OF X  IS    1.011225

   TRAY   MM PRESS    TEMP  F    MOLS VAPOR   LIQUID MOLS
     1      443.0     374.55     289.84      74.00
                    X( 1) =   .000011            Y( 1) =   .000024
                    X( 2) =   .004184            Y( 2) =   .007124
                    X( 3) =   .009304            Y( 3) =   .013158
                    X( 4) =   .283681            Y( 4) =   .352266
                    X( 5) =   .121621            Y( 5) =   .152685
                    X( 6) =   .040547            Y( 6) =   .043617
                    X( 7) =   .189221            Y( 7) =   .195815
```

Common Storage:

All dimensioned variables are stored in labeled common storage blocks. The labels and variables are as follows:

PAGE1 is used in both the main program and the subroutine, TOMSOL. This contains the variable COEFF (50, 4).

PAGE2 is used in the main program only. This contains the variables, V(50), X(50, 12), Z(12), CHV(12), CPL(12).

PAGE3 is used in the main program only. This contains the variables. HVAP(50), HLIQ(50), LIQ(50), TRAY(50).

PAGE4 is used in the main program and the subroutine, EK, to find the K values. This contains the variables, MMHG(50), DIFK (50, 12), K(50, 12).

PAGE5 is used in the main program and the subroutine, EK, to find the K values. This contains the variables, A(12), B(12), CC(12), TEMP(50).

Subroutines:

Two short subroutines are included with this program.

TOMSOL(N) - solves the tridiagonal matrix.

EK(N,NC) - determines K values and the differentials of K with respect to temperature.

Program Logic:

Data are read in and initial values are assigned by statements APDS0430 to APDS0920. Statements APDS0000 to APDS0420 are a description of how to use the program.

Statement APDS0930 is the start of the iteration. It calls the subroutine to determine K values. Statements APDS0940 and APDS0950 are to halt the iteration if an excessive number of iterations is required.

Statements APDS0960 to APDS1440 are solving the material balance equations and normalizing the compositions.

Statements APDS1450 to APDS1580 are adjusting the temperature profile for a new iteration.

Statements APDS1590 to APDS1890 are making the energy balances.

Statements APDS1900 to APDS2260 are the output section with the exception that statements APDS2160 to APDS2200 are checking to see if another run is going to be made.

Convergence is checked in statements APDS13[illegible] to APDS1440. If convergence has not been obtained the temperature and vapor profiles are adjusted and the program cycles to statement APDS0930 to start a new mass balance.

A listing of the main program is given in Table 5. Table 6 lists the subroutine EK. The subroutine TOMSOL is listed in Table 7. Table 8 lists data for a trial run. The results of this trial run are given in Table 9.

Table 5

Main Program

```
C     PROGRAM APDIST   BY L. L. HOVEY  UNIVERSITY OF WYOMING           APDS0000
C     AMUNDSEN-PCNTINEN METHOD TO DESIGN DISTILLATION TOWER SPLIT      APDS0010
C     THIS PROGRAM REQUIRES THE INPUT OF N (THE TOTAL NUMBER OF        APDS0020
C     TRAYS) WHICH MUST BE BETWEEN 1 AND 49 AND INCLUDES THE           APDS0030
C     REBOILER.  THESE ARE TRAYS AT 100  EFFICIENCY.                   APDS0040
C     M (THE NUMBER CF TRAYS BELOW THE FEED TRAY) MUST BE GIVEN        APDS0050
C     AND MUST FALL IN THE RANGE 2 TO 47.  NC (THE NUMBER OF           APDS0060
C     COMPONENTS) MUST BE GIVEN AND MUST FALL IN THE RANGE 1 TO        APDS0070
C     12.  TOPP (THE CCLUMN TOP PRESSURE IN MM HG.) MUST BE GIVEN      APDS0080
C     OR IT WILL BE ASSIGNED THE VALUE OF 760 BY THE PROGRAM.          APDS0090
C     PDPTR (THE PRESSURE DROP PER TRAY IN MM HG.) MUST BE GIVEN.      APDS0100
C     ERROR (THE CONVERGENCE LIMIT FOR THE COMPOSITION ON ANY          APDS0110
C     TRAY) MUST BE GIVEN OR THE PROGRAM WILL ASSIGN A VALUE OF        APDS0120
C     0.01 MOLE FRACTICN.  CYCLE (THE MAX NUMBER OF CYCLES             APDS0130
C     WHICH WILL BE TRIED) MUST BE SPECIFIED OR A VALUE OF 20 WILL     APDS0140
C     BE ASSIGNED.  NIND IS AN INDEX WHICH WILL CAUSE ALL TRAY         APDS0150
C     COMPOSITIONS TO BE TYPED OUT ON UNIT IOUT3 WHEN                  APDS0160
C     IT HAS A NONZERO VALUE.  THE ABOVE 8 ITEMS ARE ON THE FIRST      APDS0170
C     DATA CARD AND ARE READ WITH A FORMAT OF (3I3,3F10.5,2I3)         APDS0180
C     FOR EACH COMPONENT THE FEED COMPOSITION, Z(I), IN MOLE           APDS0190
C     FRACTION, THE CONSTANTS FOR VAPOR PRESSURE TO FIT THE EQUATION   APDS0200
C     LN (P) = A + B/T + CC/(T*T)  WHERE P IS IN MM HG., AND T         APDS0210
C     IS IN DEGREES KELVIN, THE HEAT OF VAPORIZATION OF THE            APDS0220
C     COMPONENT, CHV(I), IN BTU PER POUND MOLE AND THE HEAT            APDS0230
C     CAPACITY OF THE LIQUID, CPL(I), FOR EACH COMPONENT IN BTU        APDS0240
C     PER POUND MOLE DEGREE F. MUST BE SUPPLIED USING THE FORMAT       APDS0250
C     (6F10.5).                                                        APDS0260
C     INDEX IS AN INDEX WHICH CAUSES THE PROGRAM TO COME BACK TO       APDS0270
C     THE DATA INPUT STATEMENTS.  IF INDEX IS 1 IT RETURNS TO THE      APDS0280
C     THIRD PORTION OF THE DATA INPUT AND RETAINS THE SAME FEED        APDS0290
C     COMPOSITION AND CTHER DATA FED  IN UP TO THIS POINT.  IF         APDS0300
C     THE INDEX IS 2 NEW FEED COMPOSITIONS AND ENTHALPY DATA AND       APDS0310
C     THE SUBSEQUENT DATA CAN BE SUPPLIED.  IF THE INDEX IS 3 IT       APDS0320
C     STARTS OVER AT THE BEGINNING OF THE PROGRAM.  ANY OTHER          APDS0330
```

```
C     VALUE FOR THE INDEX WILL CAUSE THE PROGRAM TO STOP AFTER           APDS0340
C     EXECUTION OF THE PROGRAM FOR THE GIVEN DATA.  ALSO THIS            APDS0350
C     THIRD PORTION OF DATA INPUT REQUIRES THE MOLES OF OVERHEAD         APDS0360
C     PER 100 MOLES OF FEED, TOP, THE MOLES OF BOTTOMS PER               APDS0370
C     100 MOLES OF FEED, BOTT, THE TEMPERATURE OF THE FEED IN            APDS0380
C     DEGREES F, TFEED, THE ENTHALPY OF THE FEED IN BTU PER              APDS0390
C     ONE POUND MOLE OF FEED, HFEED, AND THE MOLES OF VAPOR GOING TO     APDS0400
C     THE CONDENSER PER 100 MOLES OF FEED, VINIT.  THE FORMAT            APDS0410
C     FOR THIS THIRD SECTION OF DATA IS (I2,5F10.5)                      APDS0420
      REAL K,MMHG,NONE,NMTWO,LIQ                                         APDS0430
      INTEGER CYCLE                                                      APDS0440
      COMMON /PAGE1/ CCEFF(50,4)                                         APDS0450
      COMMON /PAGE2/ V(50),X(50,12),Z(12),CHV(12),CPL(12)                APDS0460
      COMMON /PAGE3/ HVAP(50),HLIQ(50),LIQ(50),TRAY(50)                  APDS0470
      COMMON /PAGE4/ MMHG(50),DIFK(50,12),K(50,12)                       APDS0480
      COMMON /PAGE5/ A(12),B(12),CC(12),TEMP(50)                         APDS0490
C     SETTING THE INPUT AND OUTPUT UNITS.  IIN IS THE DATA INPUT         APDS0500
C     UNIT.  IOUT IS THE OUTPUT UNIT ERROR MESSAGES WILL APPEAR          APDS0510
C     ON.  IOUT1 IS THE UNIT THE MAIN SOLUTION WILL APPEAR ON.           APDS0520
C     IOUT2 IS THE UNIT WHICH GIVES THE UNADJUSTED SUM OF LIQUID         APDS0530
C     MOLE FRACTIONS FOR UNCONVERGED TRAYS.  IOUT3 IS THE UNIT           APDS0540
C     WHICH HAS INDIVIDUAL TRAY COMPOSITIONS FOR THE CASE OF             APDS0550
C     NIND HAVING A NONZERO VALUE.                                       APDS0560
      DATA IIN/5/                                                        APDS0570
      DATA IOUT/6/                                                       APDS0580
      DATA IOUT1/7/                                                      APDS0590
      DATA IOUT2/8/                                                      APDS0600
      DATA IOUT3/9/                                                      APDS0610
      NRUN=0                                                             APDS0620
      INDEX=0                                                            APDS0630
      NFLAG=0                                                            APDS0640
    4 READ (IIN,100) N,M,NC,TOPP,PDPTR,ERROR,CYCLE,NIND                  APDS0650
      WRITE (IOUT1,121)                                                  APDS0660
C     CHECKING FOR RANGE AND ASSIGNING UNASSIGNED VALUES.                APDS0670
```

```
      IF (NC.LE.0.OR.NC.GT.12) GO TO 510                                APDS0680
      IF (N.GT.49.OR.N.LE.0) GO TO 511                                  APDS0690
      IF (M.GT.47.OR.M.LT.2) GO TO 512                                  APDS0700
      IF (CYCLE.LE.0) CYCLE=20                                          APDS0710
      IF (TOPP.EQ.0) TOPP=760.                                          APDS0720
      IF (ERROR.EQ.0) ERROR=0.01                                        APDS0730
    3 DO 1 I=1,NC                                                       APDS0740
      READ (IIN,102) Z(I),A(I),B(I),CC(I),CHV(I),CPL(I)                 APDS0750
    1 WRITE (IOUT1,122) I,Z(I),A(I),B(I),CC(I),CHV(I),CPL(I)            APDS0760
   10 READ (IIN,101) INDEX,TOP,BOTT,TFEED,HFEED,VINIT                   APDS0770
      NRUN=NRUN+1                                                       APDS0780
      WRITE (IOUT1,123) NRUN,N,M,ERROR,TFEED                            APDS0790
      NBILL=0                                                           APDS0800
      NCONV=0                                                           APDS0810
      NN=N+1                                                            APDS0820
      MMM=M+2                                                           APDS0830
      NM=N-1                                                            APDS0840
      FEED=100.                                                         APDS0850
      DO 2 I=1,NN                                                       APDS0860
      TN=NN-I                                                           APDS0870
      MMHG(I)=TOPP+PDPTR*(TN)                                           APDS0880
      V(I)=VINIT                                                        APDS0890
      IF (NFLAG.EQ.1) GO TO 2                                           APDS0900
      TEMP(I)=TFEED                                                     APDS0910
    2 CONTINUE                                                          APDS0920
   11 CALL EK(N,NC)                                                     APDS0930
      NBILL=NBILL+1                                                     APDS0940
      IF (NBILL.GT.CYCLE) GO TO 99                                      APDS0950
C     SETTING UP OF A COEFF. MATRIX                                     APDS0960
      DO 75 L=1,NC                                                      APDS0970
      DO 20 I=1,NN                                                      APDS0980
      DO 20 J=1,4                                                       APDS0990
   20 COEFF(I,J)=0.0                                                    APDS1000
      DO 25 I=2,M                                                       APDS1010
      COEFF(I,2)=-V(I-1)-BOTT-V(I)*K(I,L)                               APDS1020
      COEFF(I,1)=V(I-1)*K(I-1,L)                                        APDS1030
   25 COEFF(I,3)=V(I)+BOTT                                              APDS1040
      COEFF(1,2)=-BOTT-V(1)*K(1,L)                                      APDS1050
      COEFF(1,3)=BOTT+V(1)                                              APDS1060
      COEFF(M+1,1)=V(M)*K(M,L)                                          APDS1070
      COEFF(M+1,2)=-V(M)-BOTT-V(M+1)*K(M+1,L)                           APDS1080
      COEFF(M+1,3)=V(M+1)-TOP                                           APDS1090
      DO 30 I=MMM,N                                                     APDS1100
      COEFF(I,1)=V(I-1)*K(I-1,L)                                        APDS1110
      COEFF(I,2)=-V(I-1)+TOP-V(I)*K(I,L)                                APDS1120
   30 COEFF(I,3)=V(I)-TOP                                               APDS1130
      COEFF(N+1,2)=-V(N)                                                APDS1140
      COEFF(N+1,1)=V(N)*K(N,L)                                          APDS1150
C     SETTING UP OF A R. H. S. MATRIX                                   APDS1160
      DO 40 I=1,NN                                                      APDS1170
   40 COEFF(I,4)=0.0                                                    APDS1180
      COEFF(M+1,4)=-FEED*Z(L)                                           APDS1190
C      NOW SINCE A SYSTEM OF SIMULTANEOUS EQUATIONS HAS BEEN FORMED     APDS1200
C      WE WILL CALL A MATRIX INVERSION SUBROUTINE TO OBTAIN THE SOLUTIONAPDS1210
      CALL TOMSOL(N+1)                                                  APDS1220
      DO 75 I=1,NN                                                      APDS1230
   75 X(I,L)=COEFF(I,1)                                                 APDS1240
C      NORMALIZING THE COMPOSITIONS ON EACH TRAY                        APDS1250
      DO 50 I=1,NN                                                      APDS1260
      TRAY(I)=0.0                                                       APDS1270
      DO 50 L=1,NC                                                      APDS1280
      IF (X(I,L).GE.0.0) GO TO 50                                       APDS1290
C     ELIMINATING NEGATIVE VALUES OF X(I,L)                             APDS1300
      X(I,L)=0.0                                                        APDS1310
   50 CONTINUE                                                          APDS1320
      NPOINT=1                                                          APDS1330
      DO 80 I=1,NN                                                      APDS1340
      SUM=0.0                                                           APDS1350
      DO 60 L=1,NC                                                      APDS1360
   60 SUM=SUM+X(I,L)                                                    APDS1370
      IF (ABS(1.0-SUM).LE.ERROR) GO TO 70                               APDS1380
      TRAY(I)=SUM                                                       APDS1390
      NPOINT=2                                                          APDS1400
   70 CONTINUE                                                          APDS1410
      DO 80 L=1,NC                                                      APDS1420
   80 X(I,L)=X(I,L)/SUM                                                 APDS1430
      IF (NPOINT.EQ.1)   GO TO 500                                      APDS1440
C     ADJUSTING THE TEMPERATURE PROFILE                                 APDS1450
      TADJA=0                                                           APDS1460
      DO 91 I=1,NN                                                      APDS1470
      PHI=0.0                                                           APDS1480
      DIFPHI=0.0                                                        APDS1490
      DO 90 L=1,NC                                                      APDS1500
      PHI=PHI+K(I,L)*X(I,L)                                             APDS1510
   90 DIFPHI=DIFPHI+X(I,L)*DIFK(I,L)                                    APDS1520
      TADJ=(1.0-PHI)/DIFPHI                                             APDS1530
      IF (TADJ.GT.100.) TADJ=100.                                       APDS1540
      IF (TADJ.LT.-100.) TADJ=-100.                                     APDS1550
      IF (ABS(TADJ).GE.20.) TADJA=100.                                  APDS1560
   91 TEMP(I)=TEMP(I)+TADJ                                              APDS1570
      IF (TADJA.GT.99.) GO TO 11                                        APDS1580
C     CALCULATION OF ENTHALPIES OF LIQUID AND VAPOR STREAMS LEAVING EACHAPDS1590
C     TRAY                                                              APDS1600
      DO 93 I=1,NN                                                      APDS1610
      HVAP(I)=0.0                                                       APDS1620
      HLIQ(I)=0.0                                                       APDS1630
      DO 93  L=1,NC                                                     APDS1640
      HVAP(I)=HVAP(I)+K(I,L)*X(I,L)*(CHV(L)+CPL(L)*TEMP(I))             APDS1650
   93 HLIQ(I)=HLIQ(I)+X(I,L)*CPL(L)*TEMP(I)                             APDS1660
      QC=V(N)*(HVAP(N)-HLIQ(N+1))                                       APDS1670
      QR=TOP*HLIQ(N+1)+BOTT*HLIQ(1)+QC-HFEED*FEED                       APDS1680
      V(1)=(BOTT*(HLIQ(1)-HLIQ(2))-QR)/(HLIQ(2)-HVAP(1))                APDS1690
      DO 94 I=2,M
   94 V(I)=(BOTT*(HLIQ(I)-HLIQ(I+1))-V(I-1)*(HVAP(I-1)-HLIQ(I)))
     1/(HLIQ(I+1)-HVAP(I))
      DENOM=HLIQ(M+2)-HVAP(M+1)
      NONE= TOP*HLIQ(M+2)+BOTT*HLIQ(M+1)-FEED*HFEED
      NMTWO=V(M)*(HVAP(M)-HLIQ(M+1))
      V(M+1)=(NONE-NMTWO)/DENOM
      DO 95 I=MMM,NM
   95 V(I)=(TOP*(HLIQ(I+1)-HLIQ(I))-V(I-1)*(HVAP(I-1)-HLIQ(I)))/
     1(HLIQ(I+1)-HVAP(I))
      DO 96 I=1,M
   96 LIQ(I+1)=BCTT+V(I)
      MM=M+1
      DO 97 I=N,MM,-1
   97 LIQ(I)=V(I-1)-TOP
      REFLUX=V(N)-TOP
      LIQ(1)=BOTT
      LIQ(N+1)=REFLUX
      V(N+1)=0.0
      IF (NBILL.LE.CYCLE) GO TO 11
   99 NCONV=1
      GO TO 500
   98 WRITE (IOUT1,115)
      DO 36 I=1,NN
      SOME=TRAY(I)
      IF (SOME.EQ.0.0) GO TO 36
      WRITE (IOUT2,116) I,TRAY(I)
   36 CONTINUE
      GO TO 31
  500 WRITE (IOUT1,110) NBILL
      IF (NCONV.EQ.1) GO TO 98
   31 IF (NIND.EQ.0) GC TO 33
      DO 32 I=1,NN
      WRITE (IOUT3,120)
      WRITE (IOUT3,111) I,MMHG(I),TEMP(I),V(I),LIQ(I)                   APDS2040
      DO 32 J=1,NC                                                      APDS2050
      YY=K(I,J)*X(I,J)                                                  APDS2060
   32 WRITE (IOUT3,112) J,X(I,J),J,YY                                   APDS2070
   33 DO 34 I=1,NN,N                                                    APDS2080
      WRITE (IOUT1,120)                                                 APDS2090
      WRITE (IOUT1,111) I,MMHG(I),TEMP(I),V(I),LIQ(I)                   APDS2100
      DO 34 J=1,NC                                                      APDS2110
      YY=K(I,J)*X(I,J)                                                  APDS2120
   34 WRITE (IOUT1,112) J,X(I,J),J,YY                                   APDS2130
      WRITE (IOUT1,113) QC,QR,BOTT                                      APDS2140
      WRITE (IOUT1,114) TOP,REFLUX                                      APDS2150
      NFLAG=0                                                           APDS2160
      IF (INDEX.EQ.1) NFLAG=1                                           APDS2170
      IF (INDEX.EQ.1) GO TO 10                                          APDS2180
      IF (INDEX.EQ.2) GO TO 3                                           APDS2190
      IF (INDEX.EQ.3) GO TO 4                                           APDS2200
      GO TO 600                                                         APDS2210
  510 WRITE (IOUT,117) NC                                               APDS2220
      GO TO 600                                                         APDS2230
  511 WRITE (IOUT,118) N                                                APDS2240
      GO TO 600                                                         APDS2250
  512 WRITE (IOUT,119) M                                                APDS2260
  600 CONTINUE                                                          APDS2270
  100 FORMAT (3I3,3F10.5,2I3)                                           APDS2280
  101 FORMAT (I2,5F10.5)                                                APDS2290
  102 FORMAT (6F10.5)                                                   APDS2300
  110 FORMAT (25H0FINAL SOLUTION REQUIRED ,I3,12H  ITERATIONS)          APDS2310
  111 FORMAT (1H ,I5,F10.1,F10.2,2F10.2)                                APDS2320
  112 FORMAT (20H                  X(,I2,3H) =,F9.6,                    APDS2330
     112H          Y(,I2,3H) =,F9.6)                                    APDS2340
  113 FORMAT (7H0  QC =,E13.6,6H  QR =,E13.6,13H  BOTTOMS ARE,          APDS2350
     1F10.6)                                                            APDS2360
  114 FORMAT (16H0  DISTILLATE IS,F10.6,11H  REFLUX IS,F11.6)           APDS2370
```

```
115 FORMAT (47H0  THIS DOES NOT REPRESENT A CONVERGED SOLUTION)        APDS2380
116 FORMAT (5H TRAY,I4,14H  SUM OF X IS ,F10.6)                        APDS2390
117 FORMAT (8H0  NC = ,I3,27H  WHICH IS OUT OF RANGE FOR               APDS2400
   113H THIS PROGRAM)                                                  APDS2410
118 FORMAT (7H0  N = ,I3,27H  WHICH IS OUT OF RANGE FOR                APDS2420
   113H THIS PROGRAM)                                                  APDS2430
119 FORMAT (7H0  M = ,I3,27H  WHICH IS OUT OF RANGE FOR                APDS2440
   113H THIS PROGRAM)                                                  APDS2450
120 FORMAT (52H0  TRAY  MM PRESS  TEMP  F   MOLS VAPOR  LIQUID MOLS)   APDS2460
121 FORMAT (13H1  INPUT DATA//20H COMP FEED MOLE   LN                  APDS2470
   148H (P) = A + B/T + CC/(T*T)   HEAT OF     LIQ HEAT//              APDS2480
   248H      FRACTION        A          B         CC    V              APDS2490
   321HAPORIZATION  CAPACITY//)                                        APDS2500
122 FORMAT (I4,F10.5,F11.4,F10.2,F10.0,F11.2,F10.2)                    APDS2510
123 FORMAT (6H1  RUN,I3,6H  WITH,I3,17H  TOTAL TRAYS AND,I3,           APDS2520
   121H BELOW THE FEED TRAY.//26HCONVERGENCE ERROR LIMIT IS,F9.5,      APDS2530
   222H AND THE FEED TEMP. IS,F8.2,10H DEGREES F)                      APDS2540
    END                                                                APDS2550
```

Table 6

Subroutine EK

```
   SUBROUTINE EK FOR USE WITH PROGRAM APDIST BY L. L. HOVEY  OF UW   KCAL0000
   SUBROUTINE EK(N,NC)                                              KCAL0010
   REAL K, MMHG                                                     KCAL0020
   COMMON /PAGE4/ MMHG(50),DIFK(50,12),K(50,12)                     KCAL0030
   COMMON /PAGE5/ A(12),B(12),CC(12),TEMP(50)                       KCAL0040
   NN=N+1                                                           KCAL0050
   DO 10 I=1,NN                                                     KCAL0060
   DO 10 J=1,NC                                                     KCAL0070
10 K(I,J)=EXP(A(J)+B(J)/((5./9.)*(TEMP(I)+460.))+CC(J)/(((5./9.)*   KCAL0080
  1(TEMP(I)+460.))**2))/MMHG(I)                                     KCAL0090
   DO 15 I=1,NN                                                     KCAL0100
   DO 15 J=1,NC                                                     KCAL0110
15 DIFK(I,J)=K(I,J)*(-B(J)/(((5./9.)*(TEMP(I)+460.))**2)-2.*CC(J)/  KCAL0120
  1(((5./9.)*(TEMP(I)+460.))**3))*(5./9.)                           KCAL0130
   RETURN                                                           KCAL0140
   END                                                              KCAL0150
```

Table 7

Subroutine TOMSOL

```
C     SUBROUTINE TOMSOL FOR USE WITH PROGRAM APDIST BY L. L. HOVEY. UW  TRID0000
      SUBROUTINE TOMSOL (N)                                             TRID0010
      COMMON /PAGE1/ COEFF(50.4)                                        TRID0020
      COEFF(1.3)=COEFF(1.3)/COEFF(1.2)                                  TRID0030
      COEFF(1.4)=COEFF(1.4)/COEFF(1.2)                                  TRID0040
      DO 5 I=2.N                                                        TRID0050
      IM1=I-1                                                           TRID0060
      COEFF(I.3)=COEFF(I.3)/(COEFF(I.2)-COEFF(I.1)*COEFF(IM1.3))        TRID0070
      COEFF(I.4)=(COEFF(I.4)-COEFF(I.1)*COEFF(IM1.4))/(COEFF(I.2)-COEFF TRID0060
     1(I.1)*COEFF(IM1.3))                                               TRID0090
    5 IF (ABS(COEFF(I.4)) .LT. 1.0E-70) COEFF(I.4)=0.0
      COEFF(N.1)=COEFF(N.4)                                             TRID0100
      NM1=N-1                                                           TRID0110
      DO 10 I=1.NM1                                                     TRID0120
      II=N-I                                                            TRID0130
      IP1=II+1                                                          TRID0140
   10 COEFF(II.1)=COEFF(II.4)-COEFF(II.3)*COEFF(IP1.1)                  TRID0150
      RETURN                                                            TRID0160
      END                                                               TRID0170
```

Table 8

Data for Trial Run

```
49 21 11  100.0       7.0        0.010     50  0                                DATA0000
 0.12          14.5501  -1555.47  -931947.  18027.0     49.5                    DATA0001
 0.14          16.6206  -3452.84  -547637.  18461.      56.9                    DATA0002
 0.01          16.7449  -3905.90  -404178.  18830.      64.3                    DATA0003
 0.21          14.0956  -1297.77 -1071880.  19051.      56.9                    DATA0004
 0.09          16.8285  -3475.84  -647160.  19003.      56.9                    DATA0005
 0.03          18.5543  -5375.14  -170757.  19285.      64.3                    DATA0006
 0.14          12.4528    -12.73 -1353720.  19483.      64.3                    DATA0007
 0.06          20.0222  -6639.81    29882.  19807.      64.3                    DATA0008
 0.04          19.1813  -5734.60  -261170.  20169.      64.3                    DATA0009
 0.11          20.1931  -6564.93   -57485.  19883.      64.3                    DATA0010
 0.05          18.9286  -5730.00  -261200.  20664.      71.7                    DATA0011
1  26.0          74.0      100.0      5963.8      156.0                         DATA0012
0  26.0          74.0      100.0      5963.8      286.0                         DATA0013
```

Table 9

Results of Trial Run

```
INPUT DATA

COMP FEED MOLE   LN (P) = A + B/T + CC/(T*T)   HEAT OF       LIQ HEAT

     FRACTION        A          B          CC    VAPORIZATION  CAPACITY


  1   .12000    14.5501   -1555.47   -931947.    18027.00      49.50
  2   .14000    16.6206   -3452.84   -547637.    18461.00      56.90
  3   .01000    16.7449   -3905.90   -404178.    18830.00      64.30
  4   .21000    14.0956   -1297.77  -1071880.    19051.00      56.90
  5   .09000    16.8285   -3475.84   -647160.    19003.00      56.90
  6   .03000    18.5543   -5375.14   -170757.    19285.00      64.30
  7   .14000    12.4528     -12.73  -1353720.    19483.00      64.30
  8   .06000    20.0222   -6639.81     29882.    19807.00      64.30
  9   .04000    19.1813   -5734.60   -261170.    20169.00      64.30
 10   .11000    20.1931   -6564.93    -57485.    19883.00      64.30
 11   .05000    18.9286   -5730.00   -261200.    20664.00      71.70
```

```
   RUN  1  WITH 49  TOTAL TRAYS AND 21 BELOW THE FEED TRAY.

CONVERGENCE ERROR LIMIT IS   .01000 AND THE FEED TEMP. IS  100.00 DEGREES F

 FINAL SOLUTION REQUIRED  14  ITERATIONS

   TRAY  MM PRESS  TEMP  F   MOLS VAPOR  LIQUID MOLS
    1     443.0     374.35    221.01     74.00
                  X( 1) =  .000052            Y( 1) =  .000111
                  X( 2) =  .011212            Y( 2) =  .019033
                  X( 3) =  .007098            Y( 3) =  .010009
                  X( 4) =  .279763            Y( 4) =  .346362
                  X( 5) =  .121014            Y( 5) =  .151443
                  X( 6) =  .040517            Y( 6) =  .043451
                  X( 7) =  .189114            Y( 7) =  .195125
                  X( 8) =  .081053            Y( 8) =  .062701
                  X( 9) =  .054036            Y( 9) =  .032794
                  X(10) =  .148598            Y(10) =  .106733
                  X(11) =  .067545            Y(11) =  .032152

   TRAY  MM PRESS  TEMP  F   MOLS VAPOR  LIQUID MOLS
   50     100.0     255.87        .00    130.00
                  X( 1) =  .461814            Y( 1) =  .532184
                  X( 2) =  .507025            Y( 2) =  .445784
                  X( 3) =  .018272            Y( 3) =  .014422
                  X( 4) =  .011209            Y( 4) =  .006471
                  X( 5) =  .001611            Y( 5) =  .000877
                  X( 6) =  .000028            Y( 6) =  .000015
                  X( 7) =  .000041            Y( 7) =  .000019
                  X( 8) =  .000000            Y( 8) =  .000000
                  X( 9) =  .000000            Y( 9) =  .000000
                  X(10) =  .000000            Y(10) =  .000000
                  X(11) =  .000000            Y(11) =  .000000

   QC =  .288269E 07  QR =  .435359E 07  BOTTOMS ARE 74.000000

   DISTILLATE IS 26.000000  REFLUX IS 130.000000
   RUN  2  WITH 49  TOTAL TRAYS AND 21 BELOW THE FEED TRAY.
CONVERGENCE ERROR LIMIT IS   .01000 AND THE FEED TEMP. IS  100.00 DEGREES F
 FINAL SOLUTION REQUIRED  20  ITERATIONS
   TRAY   MM PRESS   TEMP  F    MOLS VAPOR  LIQUID MOLS
    1      443.0     374.68     343.14     74.00
                   X( 1) =   .000004               Y( 1) =  .000009
                   X( 2) =   .001835               Y( 2) =  .003131
                   X( 3) =   .008391               Y( 3) =  .011890
                   X( 4) =   .284642               Y( 4) =  .354173
                   X( 5) =   .122022               Y( 5) =  .153516
                   X( 6) =   .040680               Y( 6) =  .043852
                   X( 7) =   .189841               Y( 7) =  .196848
                   X( 8) =   .081365               Y( 8) =  .063290
                   X( 9) =   .054244               Y( 9) =  .033113
                   X(10) =   .149170               Y(10) =  .107763
                   X(11) =   .067805               Y(11) =  .032464
   TRAY   MM PRESS   TEMP  F    MOLS VAPOR  LIQUID MOLS
   50      100.0     255.76         .00    260.00
                   X( 1) =   .457042               Y( 1) =  .525326
                   X( 2) =   .528062               Y( 2) =  .463090
                   X( 3) =   .014521               Y( 3) =  .011433
                   X( 4) =   .000335               Y( 4) =  .000193
                   X( 5) =   .000041               Y( 5) =  .000022
                   X( 6) =   .000001               Y( 6) =  .000000
                   X( 7) =   .000001               Y( 7) =  .000000
                   X( 8) =   .000000               Y( 8) =  .000000
                   X( 9) =   .000000               Y( 9) =  .000000
                   X(10) =   .000000               Y(10) =  .000000
                   X(11) =   .000000               Y(11) =  .000000
   QC =  .528657E 07  QR =  .675970E 07  BOTTOMS ARE 74.000000
   DISTILLATE IS 26.000000  REFLUX IS 260.000000
 *STOP* 0
```

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Figure 2. Flow Diagram of General Program Structure 357

Technical Description

Two classical approaches to the solution of multicomponent stage-by-stage distillation calculations have been in use since 1933. In the Lewis-Matheson method,[1] the number of required theoretical stages is determined for a specified split of two key components and a reflux ratio greater than the minimum. In the Thiele-Geddes method,[2] the number of theoretical stages, feed-stage location, and the reflux ratio are specified, together with the fraction of the total feed that is to be taken overhead as net distillate. The split of each component is then computed. Both methods involve tedious iterative calculations. Thus, much effort has been expended in writing digital-computer programs for making the computations. Implementation of the Thiele-Geddes method on the digital computer has been more successful than implementation of the Lewis-Matheson method, largely because of convergence difficulties with the latter approach. WHENDI is a program for making Thiele-Geddes-type calculations using a matrix formulation originally applied by Amundson and Pontinen[3] and further extended and refined by Wang and Henke.[4] Rigorous material and energy balances are made around each theoretical stage.

A typical problem statement, which is a modification of one presented by Amundson and Pontinen, follows.[5] Two identical bubble-point feeds at 213.93°F, to be sent to a distillation column operating at 250 psia, are each to consist of:

Component	*lbmoles/hr*	*Mole Fraction*
ethane	1.5	0.03
propane	10.0	0.20
n-butane	18.5	0.37
n-pentane	17.5	0.35
n-hexane	2.5	0.05
	50.0	1.00

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[1] W. K. Lewis and G. L. Matheson, *Ind. Eng. Chem.*, *24* (1932), 444.
[2] E. W. Thiele and R. L. Geddes, *Ind. Eng. Chem.*, *25* (1933), 289.
[3] N. R. Amundson and A. J. Pontinen, *Ind. Eng. Chem.*, *50* (1958), 730.
[4] J. C. Wang and G. E. Henke, *Hydrocarbon Processing*, *45*, 8 (1966), 155.
[5] The solution to this problem is given below in the section entitled "Sample Problem."

The distillation column is to contain the equivalent of 16 equilibrium stages, including a partial condenser and a partial reboiler. An external reflux rate of 150 lbmoles/hr of saturated liquid is to be used. The feeds will be sent to stages 8 and 9 (numbered down from the top). A liquid sidestream of 3 lbmoles/hr is to be withdrawn from stage 3 and a vapor sidestream of 37 lbmoles/hr from stage 13. Heat will be transferred away from stage 3 at the rate of 200,000 Btu/hr. The vapor-distillate rate will be 20 lbmoles/hr, yielding an external reflux ratio of 7.5. The Wang-Henke method is to be used for calculating products and column-interior temperatures, vapor/liquid traffic, and vapor/liquid compositions for each theoretical stage.

The mathematical formulation based on a theoretical stage model is shown in Figure 1. Each interior stage can accept up to one feed stream and can produce up to one vapor sidestream and one liquid sidestream. Heat may be transferred to or from an interior stage. The governing equations for each stage, as given by Wang and Henke, consist of:[6]

1. overall material balances,
2. component material balances,
3. component equilibrium relationships in terms of K values,
4. mole-fraction sums (vapor or liquid),
5. heat balances.

Thus, for each stage, with the feed (if any) completely specified, with the heat-transfer rate (if any) specified, and with vapor- and/or liquid-sidestream total flow rates (if any) specified, there exist 3 + 2C equations, where C equals the number of chemical species, in 3 + 2C unknowns; namely,

$x_{i,j}$ = equilibrium liquid mole fractions,

$y_{i,j}$ = equilibrium vapor mole fractions,

L_j = liquid flow rate from one stage to an adjacent stage,

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[6] The equations for the partial-reboiler and condenser stages may differ from those for the internal stages.

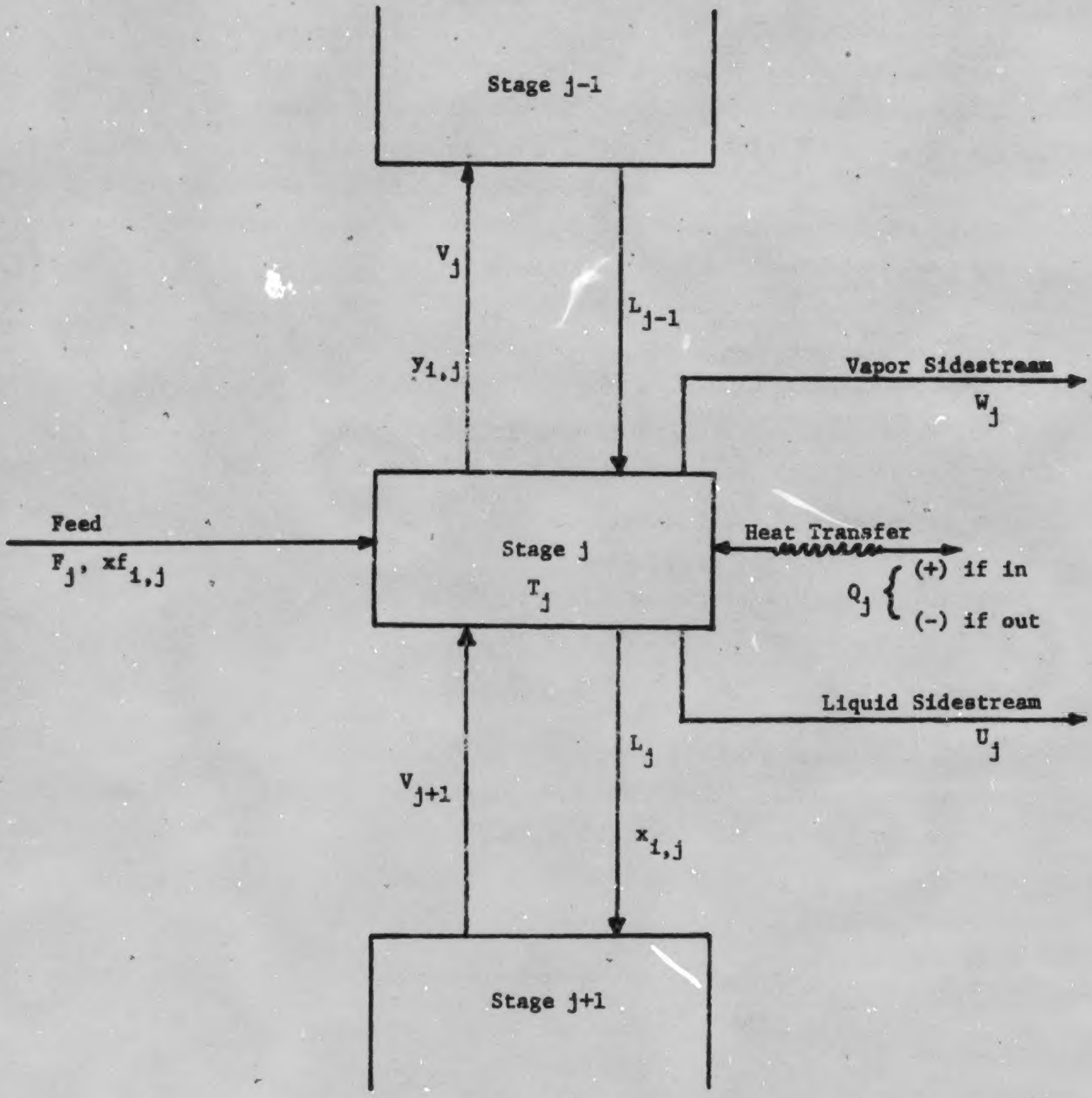
Stage j-1
V_j
$y_{i,j}$
L_{j-1}
Vapor Sidestream
W_j
Feed
F_j, $xf_{i,j}$
Stage j
T_j
Heat Transfer
Q_j
(+) if in
(-) if out
Liquid Sidestream
U_j
V_{j+1}
L_j
$x_{i,j}$
Stage j+1

FIGURE 1. THEORETICAL STAGE MODEL

V_j = vapor flow rate from one stage to an adjacent stage,

and

T_j = stage equilibrium temperature,

where i refers to the chemical species, i = 1 to C, and j refers to the stage number, j = 1 to N.

By combining the first three types of governing equations listed above, a set of C nonlinear algebraic matrix equations is obtained. The equations are linearized by use of assumed values of V_j and T_j and then solved for the liquid-phase mole fractions, $x_{i,j}$, by means of a modified Gauss elimination scheme that overcomes the deficiencies of some previous methods in that it does not produce small values from differences between large numbers nor does it produce negative mole fractions. In general, the mole fractions, $x_{i,j}$, for a given stage do not sum to 1.0 and, thus, are normalized. A new set of stage temperatures, T_j, is then computed from the component equilibrium relationships in the form of bubble-point equations. This iterative calculation utilizes Muller's method,[7] which is claimed to be superior to the Newton-Raphson or false-position iterative methods. A new set of vapor-rate values, V_j, is then computed from the heat-balance equations.

The entire calculational procedure for the distillation column is repeated until the differences between successive sets of computed stage temperatures satisfy the overall convergence criterion,

$$\sum_{j=1}^{N} (\Delta T_j)^2 \leq 0.01\ N.$$

The somewhat arbitrary value of 0.01 may be changed if desired. The assumed values of V_j and T_j for each column iteration after the first one are the calculated values from the previous iteration (successive substitution technique). To initiate the first column iteration, a linear temperature profile is assumed on the basis of estimates of the overhead and bottoms temperatures; and vapor rates are calculated on the basis of the assumption of constant molal overflow.

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[7] D. E. Muller, *Math. Tables Aids Comput.*, *10* (1956), 205.

In general, WHENDI converges to a successful solution unless the specifications result in zero or negative vapor/liquid traffic--*e.g.*, reflux completely vaporizes or the boilup completely condenses before reaching the feed plate--or unless stage temperatures correspond to values outside the range of validity of the physical-property correlations utilized. The K values are computed for each chemical species from a cubic polynomial in the temperature:

$$K_{i,j} = \alpha_i + \beta_i T_j + \gamma_i T_j^2 + \delta_i T_j^3. \tag{1}$$

The liquid and vapor enthalpy values for each stream are computed from

$$h = \sum_{i=1}^{C} h_i x_i, \tag{2}$$

where

$$h_i = a_i + b_i T + c_i T^2, \tag{3}$$

and from

$$H = \sum H_i y_i, \tag{4}$$

where

$$H_i = A_i + B_i T + C_i T^2. \tag{5}$$

Values of the coefficients in Equations 1, 3, and 5 must be supplied by the user for the particular chemical species and the column operating pressure.

Numerous examples of distillation calculations exist in the literature. Many of the general sources are referenced by King.[8] Examples, complete with the necessary physical-property polynomial-equation coefficients are available.[9,10,11] For distillation problems in which they are not already available, the physical-property polynomial-equation coefficients may be readily obtained by means of standard curve-fitting techniques[12] by use of analytical, graphical, or tabular physical-property data or correlations.

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[8] C. J. King, *Separation Processes* (New York: McGraw-Hill Book Co., 1971), pp. 493, 541.

[9] W. N. Lyster *et al.*, *Petroleum Refiner*, *38*, 6 (1959), 221.

[10] *Ibid.*, 10 (1959), 139

[11] Amundson and Pontinen, *loc. cit.*

In its present form, WHENDI is restricted to feeds and distillates that are either liquid or vapor (not those that are partially vaporized).

Educational Aspects

WHENDI may be used in any course that covers the principles of multicomponent distillation. For introductory courses, the program can afford the student the opportunity to solve one or more simple distillation problems. Examples can be chosen to illustrate the degree to which deviations can occur from the classical constant-relative-volatility and constant-molal-overflow assumptions and the extent to which non-key components may distribute.

In more advanced equilibrium-stage courses, a variety of more difficult problems may be assigned, involving, for example,

1. the degree to which a pure component can be obtained as a sidestream,
2. the effect of using an intercooler to produce supplementary reflux at a higher temperature than that of the overhead condenser or that of using a side reboiler to generate a portion of the stripping vapor at a temperature level lower than that of the bottoms reboiler,
3. the effect of feed entry point for multiple-feed cases.

While the program may be used as is for a variety of problems, it may be desirable to assign problems involving modifications to the program; *e.g.*,

1. addition of a feed flash subroutine to permit applications involving partially vaporized feeds,
2. modification of the overhead-condenser equations to permit the generation of separate vapor and liquid distillate products,

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[12] B. Carnahan, H. A. Luther, and J. O. Wilkes, *Applied Numerical Methods* (New York: John Wiley and Sons, Inc., 1969), chap. 1.

3. addition of a subroutine to accelerate the convergence of the column iterations instead of relying on successive substitution with respect to V_j and T_j,

4. replacement of the polynomial K-value treatment by a self-contained K-value calculation method, such as the Chao-Seader,[13] Lee-Edmister,[14] or Prausnitz-Chueh[15] methods.

Available textbooks, particularly King's,[16] suggest a number of other possible interesting problems and/or program modifications that might be attempted.

At least two one-hour lectures are required to present the theory of the Wang-Henke method. An additional one-hour lecture should be used to discuss the results of the first problem assignment.

Program Description

General Structure, Limitations, and History

WHENDI consists of a main driver program, nine subroutines, and two function subprograms (FEEDH and EQUILK). The overall communication scheme, the interrelationships among and the purposes of the main driver program and the subprograms, are shown in Figure 2. Besides handling all input and output tasks, the main driver program sets up the column iterations, normalizes the $x_{i,j}$ values, computes each L_j profile, and checks convergence of the column iterations. Successive cases using the same physical-property constants are automatically attempted until an end-of-file is reached (no more data cards). Two blocks of labeled common are used. BL0CK1 is common to the main driver program and to all the subprograms. It contains mainly input and output variables. BL0CK2 is common to HEAT, QDUTY, and VAP0R. It contains computed stream molal enthalpies.

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[13] K. C. Chao and J. D. Seader, *AIChE J.*, *7* (1961), 598.

[14] B. Lee and W. C. Edmister, *ibid.*, *17* (1971), 1412.

[15] J. M. Prausnitz and P. L. Chueh, *Computer Calculations for High Pressure Vapor-Liquid Equilibria* (Englewood Cliffs, N. J.: Prentice-Hall, Inc., 1968).

[16] King, *op. cit.*

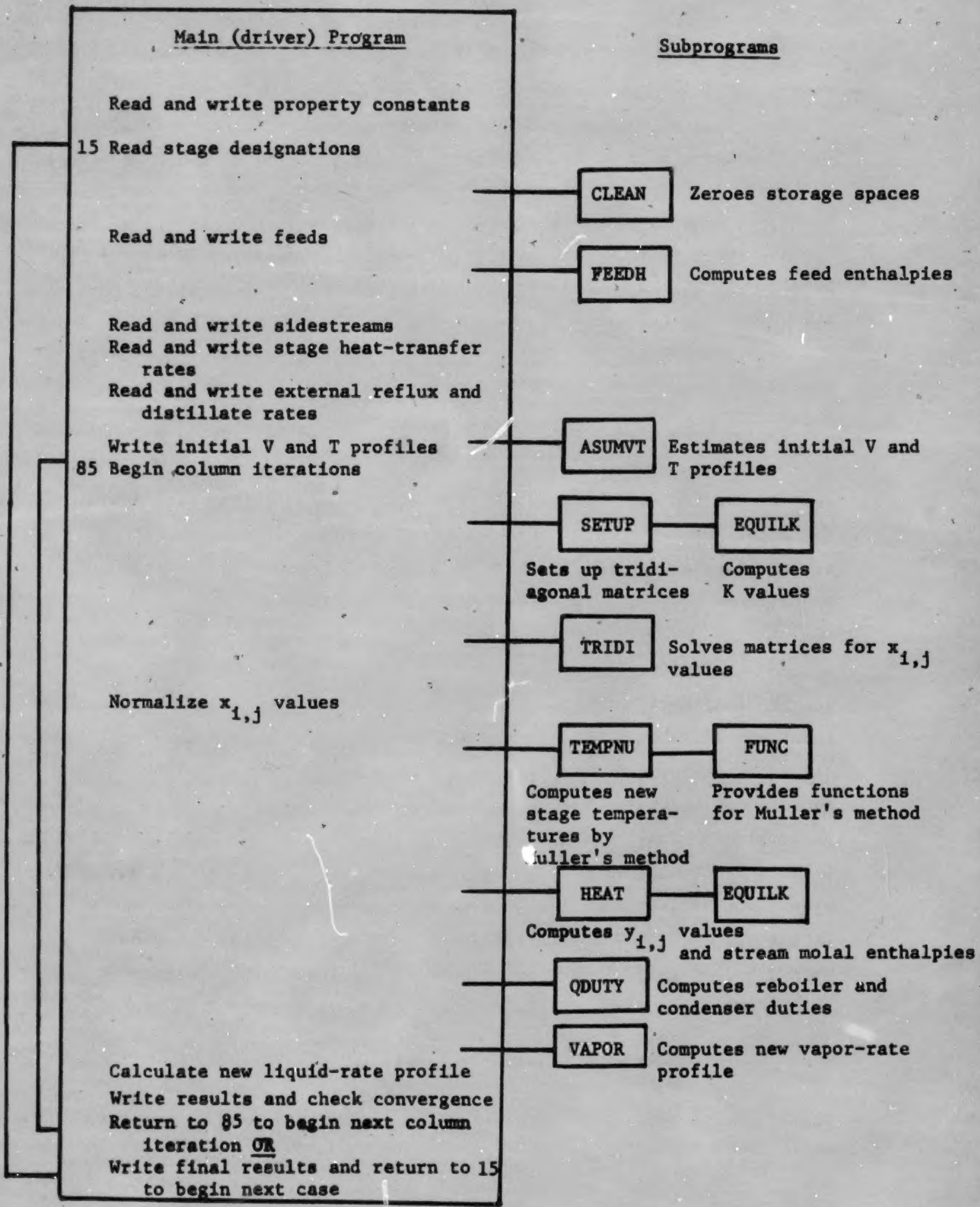
Main (driver) Program
Read and write property constants
15 Read stage designations
Read and write feeds
Read and write sidestreams
Read and write stage heat-transfer rates
Read and write external reflux and distillate rates
Write initial V and T profiles
85 Begin column iterations
Normalize $x_{i,j}$ values
Calculate new liquid-rate profile
Write results and check convergence
Return to 85 to begin next column iteration OR
Write final results and return to 15 to begin next case
Subprograms
CLEAN
Zeroes storage spaces
FEEDH
Computes feed enthalpies
ASUMVT
Estimates initial V and T profiles
SETUP
EQUILK
Sets up tridiagonal matrices
Computes K values
TRIDI
Solves matrices for $x_{i,j}$ values
TEMPNU
FUNC
Computes new stage temperatures by Muller's method
Provides functions for Muller's method
HEAT
EQUILK
Computes $y_{i,j}$ values and stream molal enthalpies
QDUTY
Computes reboiler and condenser duties
VAPOR
Computes new vapor-rate profile

FIGURE 2. FLOW DIAGRAM OF GENERAL PROGRAM STRUCTURE

The chief limitations of the program are:

1. a maximum of 20 chemical components;
2. a maximum of 100 equilibrium stages, including the partial reboiler and the condenser (the condenser is numbered as the first stage even if it is a total condenser);
3. a maximum of 15 iterations for converging the bubble-point calculations (this limit, NBPI, is set in a DATA statement in the main driver program and may be changed if desired); a maximum of NCI column iterations (if NCI is not specified in the input data, a value of 15 is used);
4. single-phase distillate and bottoms products and single-phase feeds.

The program was written in FORTRAN IV in 1968 for use on a Univac 1108. It has been used successfully every year since then. The normal system of units employed includes °F, Btu/hr, lbmoles/hr, Btu/lbmole, and psia. Stages are numbered down from the top. The condenser is always stage 1, and the reboiler is always the last stage. Feeds and sidestreams are not permissible at these two stages.

COMMON/BLOCK1

Symbol	*Type*	*Description and Usual Symbol*
A	real	Coefficients of tridiagonal matrix
B	real	Bottoms-product flow rate
D	real	Distillate rate
F	real	Feed rate, F
HF	real	Feed molal enthalpy
HLCNST	real	Coefficients of liquid-enthalpy equation
HVCNST	real	Coefficients of vapor-enthalpy equation
IC	integer	Total number of chemical components, C
JS	integer	Total number of theoretical stages (including partial reboiler and condenser, N
KCONST	real	Coefficients of polynomial K-value equation

P	real	Column operating pressure
Q	real	Heat-transfer rate to or from a stage, Q
R	real	External reflux-to-distillate ratio
T	real	Equilibrium-stage temperature, T
TB	real	Initial estimate of bottoms temperature
TD	real	Initial estimate of distillate temperature
TLØW	real	Lower limit of temperature for physical-property correlations
TF	real	Feed temperature
THI	real	Upper limit of temperature for physical-property correlations
U	real	Liquid-sidestream flow rate, U
V	real	Vapor flow rate leaving a stage to go to an adjacent stage
W	real	Vapor-sidestream flow rate, W
X	real	Liquid-phase mole fractions, x
XF	real	Feed mole fractions, xf
Y	real	Vapor-phase mole fractions, y
Z	real	Normalized liquid-phase mole fractions

The FØRTRAN symbols for physical-property coefficients are related to the usual symbols given in Equations 1, 3, and 5 as follows:

KCØNST(1,JK) = α_i HLCNST(1,JK) = a_i HVCNST(1,JK) = A_i
KCØNST(2,JK) = β_i HLCNST(2,JK) = b_i HVCNST(2,JK) = B_i
KCØNST(3,JK) = γ_i HLCNST(3,JK) = c_i HVCNST(3,JK) = C_i
KCØNST(4,JK) = δ_i

CØMMØN/BLØCK2

Symbol	*Type*	*Description*
HL	real	Liquid molal enthalpy
HV	real	Vapor molal enthalpy

The above common-block variables are not repeated in program-variable lists to follow.

Main (Driver) Program

Principal variables:

Symbol	*Type*	*Description and Usual Symbol*
ADD	real	Sum of liquid-phase mole fractions
DPHASE	integer	Distillate-phase condition (1 = vapor, 2 = liquid)
JF	integer	Feed-stage number
JP	integer	Feed-phase condition (1 = vapor, 2 = liquid)
JQ	integer	Heated- or cooled-stage number
JSL,JSV	integer	Liquid- and vapor-sidestream stage numbers
K1	integer	Column iteration number
KP	integer	Frequency of printout for results of column iteration
L	real	Liquid flow rate leaving a stage to go to an adjacent stage
LUIN	integer	Logical unit number for input device (card reader); preset to 5 in a DATA declaration
LU0UT	integer	Logical unit number for output device (printer); preset to 6 in a DATA declaration
NBPI	integer	Maximum number of bubble-point iterations; preset to 15 in a DATA declaration
NC	integer	Case number
NCI	integer	Maximum number of column iterations; set at 15 if not specified
N0F	integer	Number of feeds
N0LS	integer	Number of liquid sidestreams
N0QS	integer	Number of heated or cooled stages other than partial reboiler or condenser
N0VS	integer	Number of vapor sidestreams
PHASE	integer	Feed-phase condition (1 = vapor, 2 = liquid)
QRATE	real	Heat-transfer rate to a stage [(-) if heated, (+) if cooled], Q
RATE	real	Liquid-sidestream flow rate, U
STD	real	Sum of the square of the differences between successive sets of stage temperatures
SUM	real	Net inflow to an upper section of the column, of feeds and/or sidestreams
SUMFD	real	Sum of feed flow rates

SUMLS	real	Sum of liquid-sidestream flow rates
SUMVS	real	Sum of vapor-sidestream flow rates
TEMP	real	Feed temperature
TAL	real	Column-iteration-convergence-criterion constant; preset to 0.01 in a DATA declaration
TØL	real	Column-iteration-convergence criterion
TS	real	Stage temperatures used to begin a column iteration
VRATE	real	Vapor-sidestream flow rate, W
XFEED	real	Feed mole fractions, xf
XFLØW	real	Feed flow rate, F

Subprograms called:

Name	*Type*	*Purpose*
CLEAN	Subroutine	Zeroes out TF, F, HF, W, U, Q, V, T, XF, X, Y, and Z arrays
FEEDH	Real Function	Computes feed molal enthalpies
ASUMVT	Subroutine	Calculates initial temperature and vapor profile on the basis of a linear interpolation between TB and TD input values and the assumption of constant molal overflow, respectively
SETUP	Subroutine	Calculates the coefficients, A, of the tridiagonal matrices that represent the linearized stage equations in terms of the liquid-phase mole fractions
TRIDI	Subroutine	Solves the tridiagonal matrices for the liquid-phase mole fraction by a modified Gauss elimination method
TEMPNU	Real Function	Computes new stage temperatures from the bubble-point equation by Muller's iterative method; number of iterations is limited to the value assigned to NBPI in the main program
HEAT	Subroutine	Computes vapor-phase mole fractions and liquid- and vapor-stream molal enthalpies
QDUTY	Subroutine	Calculates heat-transfer rates for the condenser and the reboiler
VAPØR	Subroutine	Computes the new vapor-rate profile from heat-balance equations

Input (each line corresponds to one card):

Group	*Data Items*	*Format*
1	IC, TLØW, THI, P, NCI[17]	I10,3F10.2,I10
2	KCØNST(1,1), KCØNST(2,1), KCØNST(3,1), KCØNST(4,1)	4E15.5
	KCØNST(1,2), KCØNST(2,2), KCØNST(3,2), KCØNST(4,2)	4E15.5
	. . . .	.
	. . . .	.
	. . . .	.
	KCØNST(1,IC),KCØNST(2,IC),KCØNST(3,IC),KCØNST(4,IC)	.
3	HVCNST(1,1), HVCNST(2,1), HVCNST(3,1)	3E15.5
	HVCNST(1,2), HVCNST(2,2), HVCNST(3,2)	3E15.5
	. . .	.
	. . .	.
	. . .	.
	HVCNST(1,IC), HVCNST(2,IC), HVCNST(3,IC)	.
4	Same as Group 3, only HLCNST instead of HVCNST	
5	NC, JS, NØF, NØVS, NØLS, NØQS, KP[18]	7I10
6	R, TB, TD, D, DPHASE	4F10.2,I10
7	JF, PHASE, TEMP, XFLØW	2I10,2F10.2
	XFEED(1), XFEED(2), ...	5F10.5
	. . . .	.
	. . . .	.
	. . . . XFEED(IC)	.
	Repeat Group 7 for other feeds, if any, up to NØF	
8[19]	JSV, VRATE	I10,F10.2
	Repeat Group 8 for other vapor sidestreams, if any, up to NØVS	

---

[17] If a value of NCI is not specified, a default value of 15 is used.

[18] If a value of KP is not specified, a default value of 10 is used.

[19] Delete group if NØVS = 0.

9[20]	JSL, RATE	I10,F10.2
	Repeat Group 9 for other liquid sidestreams, if any, up to NØLS	
10[21]	JQ, QRATE	I10,F15.5
	Repeat Group 10 for other stages that are heated or cooled, if any, up to NØQS	

Order of chemical species must be consistent and is usually in descending volatility. Multiple cases may be run using the same components and the same physical-property constants by repeating data-card groups 5 through 10 as many times as desired.

Output:

All input data and initial T and V profiles are printed. For each column iteration, the convergence factor, STD, is compared with the tolerance factor, TØL. At the conclusion of the final column iteration or when NCI is reached, a product summary and the following interior quantities are printed for each stage: T, V, L, x_i, and y_i. In addition, the condenser duty and reboiler duty are printed. The results from intermediate column iterations may be obtained by setting KP to a value greater than 0 and less than NCI. For example, KP=2 in the data input will cause the results of iterations 2, 4, 6, etc., to be printed, until convergence is achieved.

Error messages:

A number of error flags and messages are provided in the main program to guide the user in the event that errors are detected. In general, the error messages are self-explanatory and are not described here. The detected errors affect the program in any one of three ways:

---

[20] Delete group if NØLS = 0.

[21] Delete group if NØQS = 0.

1. allow the case to proceed,
2. terminate the case and proceed to the next case,
3. terminate the program.

Input values of the physical-property-correlation coefficients are not tested for possible errors. Instead, values of the component physical properties are computed at the mid-temperature of the valid range and are printed out with the coefficients so that the user can scrutinize them.

The variables defined above are not repeated if they appear in the subprograms discussed below. If a subprogram contains no new principal variables, does not call other subprograms, and contains no complicated algorithms, it is not discussed below.

Subroutine SETUP

This subroutine computes the coefficients, A, of the tridiagonal matrix for each chemical component at a time. The two-dimensional A array here replaces the one-dimensional A, B, C, and D arrays used in the Wang-Henke article. Thus, including the constant vector, each component matrix has the dimensions, JS by (JS + 1). The matrix equation is given as Equation 10 in the Wang-Henke article, with coefficients defined in subsequent equations in that article. The derivation of these equations is a good student exercise in advanced courses. Since WHENDI does not allow for a combined vapor and liquid distillate, Equation 11 in the Wang-Henke article is rewritten as

$$B_1 = -\left(V_1 K_{i1} + V_2 - V_1\right).$$

Also, the quantity, D_j, in the Wang-Henke article is given by the relationship,

$$D_j = -F_j z_{ij}.$$

Principal variables:

Symbol	*Type*	*Description*
JMINS	integer	Number of intermediate stages
M1	integer	Number of columns in the matrix
NSTEP	integer	Related to a particular column of the matrix

Subprograms called:

Name	*Type*	*Purpose*
EQUILK	Real Function	Computes K values at designated temperature for designated chemical species

Subroutine TRIDI

This subroutine solves the tridiagonal matrix for the x_j values for a particular component by means of a modified Gauss elimination method, described in the Wang-Henke article on pages 157-158.

Principal variables:

Symbol	*Type*	*Corresponding Symbol in Wang-Henke Article*
P(1)	real	p_1
QA(1)	real	q_1
P(J1)	real	p_j
QA(J1)	real	q_j

Function TEMPNU

This function utilizes Muller's iterative method, as described on page 160 of the Wang-Henke article, to compute new stage temperatures from the bubble-point equation. The method requires three starting values of the stage temperature, which are provided in the function from the following relationships, which are written in terms of absolute temperatures in the program:

$$XT(1) = 0.8\ T_{old},$$

$$XT(2) = 1.2\ T_{old},$$

$$XT(3) = T_{old}$$

The number of maximum iterations allowed for convergence by Muller's method is NBPI, which is set in a DATA declaration in the main program. The calculation of the actual bubble-point equation functions,

$$f(T) = \sum K_i x_i - 1.0,$$

is made in Subroutine FUNC, which is called by TEMPNU.

Principal variables:

Symbol	*Type*	*Corresponding Symbol in Wang-Henke Article*
DELTA	real	$1 + d_{k-1}$
DIFF	real	$z_{k-1} - z_{k-2}$
DI	real	Argument of the radical in Equation 22a
F1	real	$f(z_{k-3})$ bubble-point-equation functions
F2	real	$f(z_{k-2})$
F3	real	$f(z_{k-1})$
G	real	b
STEP	real	d_{k-1}
XT	real	z

Subprogram called:

Name	*Type*	*Purpose*
FUNC	Subroutine	Computes F1, F2, and F3

Miscellaneous Comments Concerning Subprograms

Both HEAT and FUNC also call EQUILK. A separate subprogram is not provided for computing component liquid and/or vapor molal enthalpies. Instead, they are calculated where required in FEEDH and HEAT.

Sample Problem

The application of WHENDI may be illustrated by obtaining the solution to the problem stated in the section, "Technical Description." This example makes use of most of the features of WHENDI. An echo print of the data is shown after the FØRTRAN program listing given below. The physical-property coefficients are those given by Amundson and Pontinen[22] except for some corrected values. These properties are valid for a temperature range of 50°F to 350°F. The feed bubble-point temperature of 213.93°F was determined by a flash program, such as FLASHC. The heat-removal specification for stage 3 is equivalent to an intercooler. Attempts are made to obtain propane-rich and n-butane-rich products by withdrawing sidestreams. A value of 3 for KP will cause intermediate results to be printed every three column iterations. A maximum of 25 column iterations is permitted by assigning this value to NCI in the input data rather than by omitting a value for NCI and, thereby, accepting the default value of 15.

The results of the calculations for the sample problem are given following the echo print of the input data, except that only one summary of intermediate results is included.

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[22] Amundson and Pontinen, *loc. cit.*

FØRTRAN Program Listing: Main Program Followed by Subprograms

```
C-----MAIN PROGRAM FOR         W H E N D I                              MAIN0001
C-----MULTICOMPONENT DISTILLATION BY THE WANG-HENKE METHOD              MAIN0002
C-----WRITTEN BY P. J. JOHANSEN AND J. D. SEADER, UNIVERSITY OF UTAH    MAIN0003
C-----LAST REVISION -   JUNE, 1972                                      MAIN0004
      REAL KCONST, L                                                    MAIN0005
      INTEGER PHASE, DPHASE, FLAG, AFLAG                                MAIN0006
      EXTERNAL EQUILK                                                   MAIN0007
      DIMENSION TS(100), XFEED(20), L(100), JP(100), PH(2),             MAIN0008
     1AK(20), HV(20), HL(20)                                            MAIN0009
      COMMON/BLOCK1/JS, IC, B, D, R, TB, TD, T(100), NBPI, NCI,         MAIN0010
     1F(100), TF(100), HF(100), XF(20, 100), Y(20, 100), Z(20, 100),   MAIN0011
     2A(100, 101), X(20,100), W(100), U(100), Q(100), V(100),           MAIN0012
     3KCONST(4, 20), HVCNST(3,20), HLCNST(3,20)                         MAIN0013
C-----ASSIGN INPUT/OUTPUT DEVICE NUMBERS,ITERATION LIMIT,  AND TOLERANCEMAIN0014
      DATA LUIN, LUOUT, NBPI, TAL/5,6,15,.01/                           MAIN0015
      DATA PH(1), PH(2)/3HVAP,3HLIQ/                                    MAIN0016
      READ (LUIN,230) IC, TLOW, THI, P, NCI                             MAIN0017
      IF (NCI .EQ. 0) NCI = 15                                          MAIN0018
      WRITE (LUOUT,225) NBPI,NCI,TAL                                    MAIN0019
      TT = (THI + TLOW)/2.                                              MAIN0020
      WRITE (LUOUT,245) P,TLOW, THI, TT                                 MAIN0021
      IF (IC .GT. 1 .AND. IC .LE. 20) GO TO 5                           MAIN0022
      WRITE (LUOUT,420)                                                 MAIN0023
      GO TO 200                                                         MAIN0024
C-----READ IN AND PRINT THE PHYSICAL PROPERTY DATA                      MAIN0025
    5 READ (LUIN,235) ((KCONST(IK,JK), IK = 1,4), JK =1, IC)            MAIN0026
      READ (LUIN, 240) ((HVCNST(IK, JK), IK = 1,3), JK = 1,IC)          MAIN0027
      READ (LUIN, 240) ((HLCNST(IK, JK), IK = 1,3), JK = 1, IC)         MAIN0028
      DO 10 JK = 1,IC                                                   MAIN0029
      AK(JK) = EQUILK(TT,JK)                                            MAIN0030
      HV(JK) = HVCNST(1,JK) + HVCNST(2,JK)*TT + HVCNST(3,JK)*TT*TT      MAIN0031
      HL(JK) = HLCNST(1,JK) + HLCNST(2,JK)*TT + HLCNST(3,JK)*TT*TT      MAIN0032
   10 CONTINUE                                                          MAIN0033
      WRITE (LUOUT,250) (JK,(KCONST(IK,JK),IK=1,4), AK(JK), JK=1,IC)    MAIN0034
      WRITE (LUOUT,255) (JK,(HVCNST(IK,JK),IK=1,3), HV(JK), JK=1,IC)    MAIN0035
      WRITE (LUOUT,260) (JK,(HLCNST(IK,JK),IK=1,3), HL(JK), JK=1,IC)    MAIN0036
C-----READ IN AND PRINT DATA FOR A CASE                                 MAIN0037
   15 READ (LUIN, 265) NC, JS, NOF, NOVS, NOLS, NOQS, KP                MAIN0038
      IF (KP .EQ. 0) KP = 10                                            MAIN0039
      IF (JS .GT. 2 .AND. JS .LE. 100) GO TO 20                         MAIN0040
      WRITE (LUOUT,430)                                                 MAIN0041
      GO TO 200                                                         MAIN0042
C-----ZERO OUT CERTAIN ARRAYS BEFORE STARTING A CASE                    MAIN0043
   20 CALL CLEAN                                                        MAIN0044
      TOL = TAL * JS                                                    MAIN0045
      READ (LUIN, 270) R, TB, TD, D, DPHASE                             MAIN0046
      WPHASE = PH(1)                                                    MAIN0047
      IF (DPHASE .EQ.2) WPHASE = PH(2)                                  MAIN0048
      WRITE (LUOUT,275) NC,IC,JS,NOF,NOVS,NOLS,NOQS,R,D,WPHASE,TD,TB    MAIN0049
      WRITE (LUOUT,280) IC                                              MAIN0050
      SUMFD = 0.0                                                       MAIN0051
      DO 35 L1 = 1, NOF                                                 MAIN0052
      READ (LUIN, 285) JF, PHASE, TEMP, XFLOW                           MAIN0053
      READ (LUIN, 290) (XFEED(L2), L2 = 1, IC)                          MAIN0054
      WPHASE = PH(1)                                                    MAIN0055
      IF (PHASE .EQ. 2) WPHASE = PH(2)                                  MAIN0056
      WRITE (LUOUT,295) JF, XFLOW, WPHASE, TEMP, (XFEED(L2), L2=1,IC)   MAIN0057
      SUMMF = 0.0                                                       MAIN0058
      DO 25 M = 1, IC                                                   MAIN0059
      SUMMF = SUMMF + XFEED(M)                                          MAIN0060
   25 CONTINUE                                                          MAIN0061
      IF (SUMMF .LT. 0.999 .OR. SUMMF .GT. 1.001) WRITE (LUOUT,435) JF  MAIN0062
      IF (SUMMF .LT. 0.999 .OR. SUMMF .GT. 1.001) WRITE (LUOUT,440)     MAIN0063
      TF(JF) = TEMP                                                     MAIN0064
      F(JF) = XFLOW                                                     MAIN0065
      JP(JF) = PHASE                                                    MAIN0066
      SUMFD = SUMFD + F(JF)                                             MAIN0067
      DO 30 L2 = 1, IC                                                  MAIN0068
      XF(L2,JF) = XFEED(L2)                                             MAIN0069
   30 CONTINUE                                                          MAIN0070
C-----COMPUTE FEED ENTHALPY                                             MAIN0071
      HF(JF) = FEEDH (PHASE, JF)                                        MAIN0072
   35 CONTINUE                                                          MAIN0073
      SUMVS = 0.                                                        MAIN0074
      SUMLS = 0.                                                        MAIN0075
      KKK = 0                                                           MAIN0076
      IF (NOVS .EQ. 0) GO TO 45                                         MAIN0077
      WPHASE = PH(1)                                                    MAIN0078
      WRITE (LUOUT, 300)                                                MAIN0079
      KKK = 1                                                           MAIN0080
      DO 40 L3 = 1, NOVS                                                MAIN0081
      READ (LUIN, 230) JSV, VRATE                                       MAIN0082
      WRITE (LUOUT, 305) JSV, VRATE, WPHASE                             MAIN0083
      IF (JSV .LT. 2 .OR. JSV .GT. (JS-1)) GO TO 200                    MAIN0084
      W(JSV) = VRATE                                                    MAIN0085
      SUMVS = W(JSV) + SUMVS                                            MAIN0086
   40 CONTINUE                                                          MAIN0087
   45 IF (NOLS .EQ. 0) GO TO 55                                         MAIN0088
      WPHASE = PH(2)                                                    MAIN0089
      IF (KKK .EQ. 0) WRITE (LUOUT,300)                                 MAIN0090
      DO 50 L4 = 1, NOLS                                                MAIN0091
      READ (LUIN, 230) JSL, RATE                                        MAIN0092
      WRITE (LUOUT, 305) JSL, RATE, WPHASE                              MAIN0093
      IF (JSL .LT. 2 .OR. JSL .GT. (JS-1)) GO TO 200                    MAIN0094
      U(JSL) = RATE                                                     MAIN0095
      SUMLS = U(JSL) + SUMLS                                            MAIN0096
   50 CONTINUE                                                          MAIN0097
   55 IF (NOQS .EQ. 0) GO TO 65                                         MAIN0098
      WRITE (LUOUT, 310)                                                MAIN0099
      DO 60 L5 = 1, NOQS                                                MAIN0100
      READ (LUIN, 315) JQ, QRATE                                        MAIN0101
      WRITE (LUOUT, 320) JQ, QRATE                                      MAIN0102
      IF (JQ .LT. 2 .OR. JQ .GT. (JS-1)) GO TO 200                      MAIN0103
      Q(JQ) = QRATE                                                     MAIN0104
   60 CONTINUE                                                          MAIN0105
   65 B = SUMFD - D - SUMVS - SUMLS                                     MAIN0106
      IF (B .LT. 0.0) WRITE (LUOUT,445) B                               MAIN0107
      IF (B .LT. 0.0) GO TO 15                                          MAIN0108
      IF (DPHASE .EQ. 1) GO TO 70                                       MAIN0109
      V(1) = 0.0                                                        MAIN0110
      GO TO 75                                                          MAIN0111
   70 V(1) = D                                                          MAIN0112
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C-----COMPUTE INITIAL TEMPERATURE AND VAPOR RATE PROFILES
   75 CALL ASUMVT(JP)
      WRITE (LUOUT,325)
      WRITE (LUOUT,330) (I, T(I), V(I), I= 1,JS)
      WRITE (LUOUT,335) KP
      DO 80 I=1,JS
      TS(I) = T(I)
   80 CONTINUE
      K2 = 0
      K1= 0
   85 K1 = K1 + 1
      K2 = K2 + 1
C-----COMPUTE MATRIX COEFFICIENTS
      DO 90 I = 1, IC
      CALL SETUP (I, EQUILK)
C-----SOLVE MATRIX FOR LIQUID MOLE FRACTIONS
      CALL TRIDI(I)
   90 CONTINUE
C-----NORMALIZE LIQUID MOLE FRACTIONS
      DO 105 KA = 1, JS
      ADD = 0.0
      DO 95 JA = 1, IC
      ADD = ADD + X(JA,KA)
   95 CONTINUE
      DO 100 JB = 1, IC
      Z(JB,KA) = X(JB,KA)/ADD
  100 CONTINUE
  105 CONTINUE
C-----COMPUTE NEW STAGE TEMPERATURES
      DO 110 J = 1, JS
      TVAL = T(J)
      T(J) = TEMPNU(TVAL, J, FLAG)
      IF (FLAG .EQ. 1) WRITE (LUOUT,450) J, NBPI, NCI, T(J)
      IF (T(J) .LT. TLOW .OR. T(J) .GT. THI) GO TO 205
C-----COMPUTE VAPOR MOLE FRACTIONS AND STREAM ENTHALPIES
      CALL HEAT (J, EQUILK)
  110 CONTINUE
C-----COMPUTE REBOILER AND CONDENSER DUTIES
      CALL QDUTY (QB, QD)
C-----COMPUTE NEW VAPOR RATE PROFILE
      CALL VAPOR (QB, QD, AFLAG, J2, ALIQ)
      IF (AFLAG .EQ. 1) GO TO 210
      IF (AFLAG .EQ. 2) GO TO 220
      IF (K2 .NE. KP .AND. K1 .NE. NCI) GO TO 140
      WRITE (LUOUT,360)
      WRITE (LUOUT,340) K1, IC
      K2 = 0
C------COMPUTE NEW LIQUID RATE PROFILE
      SUM = 0.0
      DO 135 I = 1, JS
      IF (I .EQ. 1) GO TO 120
      SUM = SUM + F(I) - W(I) - U(I)
      IF (I .EQ. JS) GO TO 115
      L(I) = V(I + 1) + SUM - D
      GO TO 125
  115 L(I) = SUM - D
      GO TO 125
  120 L(1) = R*D
C-----COMPUTE SUM OF LIQUID MOLE FRACTIONS
  125 ADD = 0.0
      DO 130 K = 1, IC
      ADD = ADD + X(K,I)
  130 CONTINUE
      WRITE (LUOUT, 345) I, T(I), V(I), L(I), (X(K, I), K = 1, IC)
      WRITE (LUOUT, 350) ADD
      WRITE (LUOUT, 355) (Y(K, I), K = 1, IC)
  135 CONTINUE
C-----CONVERGENCE TEST
  140 STD = 0.0
      DO 145 J = 1, JS
      DIFF = T(J) - TS(J)
      TS(J) = T(J)
      STD = STD + DIFF * DIFF
  145 CONTINUE
      IF (STD .GT. TOL .AND. K1 .LT. NCI) WRITE (LUOUT,365) K1,STD,TOL
      IF (STD .GT. TOL .AND. K1 .LT. NCI) GO TO 85
      IF (STD.LE.TOL)  GO TO 150
      IF (K1 .EQ. NCI) WRITE (LUOUT,375) NCI
      GO TO 155
  150 WRITE (LUOUT, 370) K1, STD, TOL
  155 WRITE (LUOUT,380) IC
      IF (DPHASE .EQ. 1) WRITE (LUOUT,385) PH(1),T(1),D,(Y(K,1), K=1,IC)
      IF (DPHASE .EQ. 2) WRITE (LUOUT,385) PH(2),T(1),D,(X(K,1), K=1,IC)
      JSS = JS - 1
      IF (NOVS .EQ. 0) GO TO 165
      DO 160 I=2,JSS
      IF (W(I) .LT. .00001) GO TO 160
      WRITE (LUOUT,390) I, PH(1), T(I), W(I), (Y(K,I), K=1,IC)
  160 CONTINUE
  165 IF (NOLS .EQ. 0) GO TO 175
      DO 170 I=2,JSS
      IF (U(I) .LT. .00001) GO TO 170
      WRITE (LUOUT,390) I, PH(2), T(I), U(I), (X(K,I), K=1,IC)
  170 CONTINUE
  175 WRITE (LUOUT,395) JS, PH(2), T(JS),B, (X(K,JS), K=1,IC)
  180 WRITE (LUOUT,400) QD,QB
  185 WRITE (LUOUT,405) IC,IC
      DO 195 I=1,JS
      IF (I.EQ.1) GO TO 190
      WRITE (LUOUT,410) I, T(I), V(I), (Y(K,I), K=1,IC)
      IF (I.EQ.JS) GO TO 195
  190 WRITE (LUOUT,415) I, T(I), L(I), (X(K,I), K=1,IC)
  195 CONTINUE
      GO TO 15
  200 WRITE (LUOUT,425)
      STOP
  205 WRITE (LUOUT,455) T(J), J, K1
      WRITE (LUOUT,460)
      STOP
  210 WRITE (LUOUT,465) V(J2), J2, K1
      WRITE (LUOUT,470)
  215 WRITE (LUOUT,480)
      GO TO 15
  220 WRITE (LUOUT,475) ALIQ, J2, K1
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      WRITE (LUOUT,470)                                                 MAIN0227
      GO TO 215                                                         MAIN0228
  225 FORMAT (1H1//////55X,11HW H E N D I//////////36X,48HMULTICOMPONENTMAIN0229
     1 DISTILLATION BY WANG-HENKE METHOD/////////30X,61HMAXIMUM NUMBER OMAIN0230
     2F ITERATIONS FOR BUBBLE-POINT CALCULATIONS = ,I3////30X,38HMAXIMUMMAIN0231
     3 NUMBER OF COLUMN ITERATIONS = ,I4////30X,54HCONSTANT FOR COLUMN IMAIN0232
     4TERATION CONVERGENCE CRITERION = ,F7.5/1H1)                       MAIN0233
  230 FORMAT (I10,3F10.2, I10)                                          MAIN0234
  235 FORMAT (4E15.5)                                                   MAIN0235
  240 FORMAT (3E15.5)                                                   MAIN0236
  245 FORMAT (//33X,54HCOEFFICIENTS OF POLYNOMIAL PHYSICAL-PROPERTY EQUAMAIN0237
     1TIONS//41X,38HPROPERTY = A + B*T + C*T**2. + D*T**3./48X,16HWITH TMAIN0238
     2 IN DEG. F///41X,11HPRESSURE = ,F8.3,6H  PSIA//41X,26HVALID TEMPERMAIN0239
     3ATURE RANGE = ,F8.2,4H TO ,F8.2,8H  DEG. F////101X,14HPROPERTY VALMAIN0240
     4UE/25X,9HCOMPONENT,8X,1HA,14X,1HB,14X,1HC,14X,1HD,11X,3HAT ,F8.2,7MAIN0241
     5H DEG. F/25X,9H---------,3X,11H-----------,4X,11H-----------,4X,11MAIN0242
     6H-----------,4X,11H-----------, 6X,18H------------------//)       MAIN0243
  250 FORMAT (10X,9HK-VALUES /(26X,I5,2X,4E15.5,6X,F15.5)/)             MAIN0244
  255 FORMAT (10X,16HVAPOR ENTHALPIES/10X,13H(BTU/LBMOLE) /(26X,I5,2X,3EMAIN0245
     115.5,21X,F15.5)/)                                                 MAIN0246
  260 FORMAT (10X,17HLIQUID ENTHALPIES/10X,13H(BTU/LBMOLE) /(26X,I5,2X,3MAIN0247
     1E15.5,21X,F15.5)/)                                                MAIN0248
  265 FORMAT (8I10)                                                     MAIN0249
  270 FORMAT (4F10.2,I10)                                               MAIN0250
  275 FORMAT (1H1//53X,11HCASE NUMBER,I10////35X,29HNO. OF CHEMICAL COMPMAIN0251
     1ONENTS = ,I5//35X,28HNO. OF THEORETICAL STAGES = ,I5//35X,15HNO. OMAIN0252
     2F FEEDS = ,I5//35X,27HNO. OF VAPOR SIDESTREAMS = ,I5//35X,28HNO. OMAIN0253
     3F LIQUID SIDESTREAMS = ,I5//35X,30HNO. OF HEAT-TRANSFER STAGES = ,MAIN0254
     4I5//35X,43HEXTERNAL REFLUX-TO-DISTILLATE MOLE RATIO = ,F15.5//35X,MAIN0255
     518HDISTILLATE RATE = ,F15.5,2X,10HLBMOLES/HR,2X,A4//35X,50HESTIMATMAIN0256
     6ED DISTILLATE AND BOTTOMS TEMPERATURES ARE ,F10.2,4H AND,F10.2,7H MAIN0257
     7DEG. F////35X,35HPARTIAL REBOILER COUNTS AS A STAGE./35X,62HCONDENMAIN0258
     8SER IS NUMBERED AS A STAGE EVEN IF DISTILLATE IS LIQUID./   35X,38MAIN0259
     9HSTAGES ARE NUMBERED DOWN FROM THE TOP./1H1)                      MAIN0260
  280 FORMAT (///32X,55HFEED, SIDESTREAM, AND HEAT-TRANSFER RATE SPECIFIMAIN0261
     1CATIONS///56X,13HHEAT-TRANSFER/23X, 9HFLOW RATE,6X,5HPHASE,5X,5HTEMAIN0262
     2MP.,8X,4HRATE/15X,5HSTAGE,2X,12H(LBMOLES/HR),2X, 9HCONDITION,2X,8HMAIN0263
     3(DEG. F),3X,8H(BTU/HR),7X,44HCOMPONENT MOLE FRACTIONS FOR COMPONENMAIN0264
     4TS 1 TO,I3/                                                       MAIN0265
     5                                                       15X,105H---MAIN0266
     6- -----------  --------  --------  ------------  -------------MAIN0267
     7---------------------------------------------------//5X,6HFEEDS /) MAIN0268
  285 FORMAT (2I10,2F10.2)                                              MAIN0269
  290 FORMAT (5F10.5)                                                   MAIN0270
  295 FORMAT (14X,I5,F15.5,4X,A4,2X,F10.2,16X,5F10.5/(70X,5F10.5 )//)   MAIN0271
  300 FORMAT (5X,12HSIDESTREAMS /)                                      MAIN0272
  305 FORMAT (14X,I5,F15.5,4X,A4/)                                      MAIN0273
  310 FORMAT (5X,14HHEAT TRANSFER,/3X,16H(-) IF TO STAGE,/3X,18H(+) IF FMAIN0274
     1ROM STAGE /)                                                      MAIN0275
  315 FORMAT (I10,F15.5)                                                MAIN0276
  320 FORMAT (15X,I5,33X,E15.5/)                                        MAIN0277
  325 FORMAT (1H1///40X,39HSTAGE TEMPERATURES AND VAPOR FLOW RATES//43X,MAIN0278
     136HUSED TO INITIALIZE COLUMN ITERATIONS///49X,11HTEMPERATURE,10X,1MAIN0279
     20HVAPOR RATE/38X,5HSTAGE,8X,8H(DEG. F),10X,12H(LBMOLES/HR)/38X,5H-MAIN0280
     3----,6X,12H------------,8X,12H------------/)                      MAIN0281
  330 FORMAT (   38X,I5,7X,F10.2,6X,F15.5)                              MAIN0282
  335 FORMAT (/9X,46HINTERMEDIATE RESULTS WILL BE PRINTED OUT EVERY,I5,2MAIN0283
     1X,17HCOLUMN ITERATIONS/)                                          MAIN0284
 340 FORMAT (40X,34HINTERMEDIATE RESULTS FOR ITERATION,I4///13X,5HTEMP.MAIN0285
     1,5X,10HVAPOR RATE,4X,11HLIQUID RATE,4X,40HLIQUID, FOLLOWED BY VAPOMAIN0286
     2R,MOLE FRACTIONS,10X,11HLIQUID MOLE/5X,5HSTAGE,2X,8H(DEG. F),2X,12MAIN0287
     3H(LBMOLES/HR),3X,12H(LBMOLES/HR),5X,15HCOMPONENTS 1 TO,I3,30X,12HFMAIN0288
     4RACTION SUM/5X,5H-----,2X,8H--------,2X,12H------------,3X,12H----MAIN0289
     5--------,3X,47H-----------------------------------------------,3X,MAIN0290
     612H------------)                                                  MAIN0291
 345 FORMAT (4X,I4,2X,F9.2,F15.5,F15.5,5F10.5/(50X,5F10.5))             MAIN0292
 350 FORMAT ( 99X,F10.5)                                                MAIN0293
 355 FORMAT  (49X,5F10.5)                                               MAIN0294
 360 FORMAT (1H1)                                                       MAIN0295
 365 FORMAT (/20X,15HAFTER ITERATION,I5,2X,31HCALCULATIONS ARE NOT CONVMAIN0296
     1ERGED./20X,38HCOLUMN ITERATION CONVERGENCE FACTOR IS,E15.5,2X,36H,MAIN0297
     2 WHICH IS GREATER THAN TOLERANCE OF,F10.5)                        MAIN0298
 370 FORMAT (/20X,15HAFTER ITERATION,I5,2X,27HCALCULATIONS ARE CONVERGEMAIN0299
     1D./20X,26HCOLUMN ITERATION FACTOR IS,F10.5,2X,33H  WHICH IS LESS TMAIN0300
     2HAN TOLERANCE OF,F10.5/20X,43HFINAL DETAILED RESULTS WILL NOW BE PMAIN0301
     3RINTED.)                                                          MAIN0302
 375 FORMAT (/20X,91HCALCULATIONS ARE NOT CONVERGED AFTER MAXIMUM NUMBEMAIN0303
     1R OF COLUMN ITERATIONS, NCI, SPECIFIED AS,I5/20X,78HDETAILED UNCONMAIN0304
     2VERGED RESULTS WILL NOW BE PRINTED SO USER CAN DETERMINE WHETHER/2MAIN0305
     30X,59HIT IS WORTHWHILE TO REPEAT CASE WITH A LARGER VALUE OF NCI.)MAIN0306
 380 FORMAT (1H1////53X,13HFINAL RESULTS//42X,36HPRODUCT STREAMS AND EXMAIN0307
     1CHANGER DUTIES//16X,4HFROM,3X,5HPHASE,5X,5HTEMP.,5X,9HFLOW RATE,8XMAIN0308
     2,24HCOMPONENT MOLE FRACTIONS/7X,6HSTREAM,2X,5HSTAGE,1X,9HCONDITIONMAIN0309
     3,1X,8H(DEG. F),3X,12H(LBMOLES/HR),6X,19HFOR COMPONENTS 1 TO,I4/7X,MAIN0310
     46H------,2X,5H-----,1X,8H--------,2X,8H--------,3X,11H-----------,MAIN0311
     53X,48H------------------------------------------------/)          MAIN0312
 385 FORMAT (4X,10HDISTILLATE,3X,2H 1,5X,A4,1X,F10.2,F15.5,5F10.5/(55X,MAIN0313
     15F10.5)/)                                                         MAIN0314
 390 FORMAT (4X,10HSIDESTREAM,2X,I3,5X,A4,1X,F10.2,F15.5,5F10.5/(55X,5FMAIN0315
     110.5)/)                                                           MAIN0316
 395 FORMAT (5X,7HBOTTOMS,4X,I3,5X,A4,1X,F10.2,F15.5,5F10.5/(55X,5F10.5MAIN0317
     1)/)                                                               MAIN0318
 400 FORMAT (20X,17HCONDENSER DUTY = ,E15.5, 8H  BTU/HR/20X,18HREBOILERMAIN0319
     1 DUTY =   ,E14.5, 8H  BTU/HR/1H1)                                 MAIN0320
 405 FORMAT (////53X,13HFINAL RESULTS//51X,19HINTERNAL CONDITIONS//27X,MAIN0321
     117HFLOWS FROM STAGES/13X,5HTEMP.,5X,10HVAPOR RATE,4X,11HLIQUID RATMAIN0322
     2E,4X,21HLIQUID MOLE FRACTIONS,19X,20HVAPOR MOLE FRACTIONS/5X,5HSTAMAIN0323
     3GE,2X,8H(DEG. F),2X,12H(LBMOLES/HR),3X,12H(LBMOLES/HR),3X,16HCOMPOMAIN0324
     4NENTS 1 TO ,I4,20X,16HCOMPONENTS 1 TO ,I4/5X,5H-----,2X,9H--------MAIN0325
     5-,2X,12H------------,3X,12H------------,2X,38H--------------------MAIN0326
     6------------------,2X,38H--------------------------------------//)MAIN0327
 410 FORMAT (5X,I4,1X,F10.2,F15.5,55X,5F8.5/(90X,5F8.5))                MAIN0328
 415 FORMAT (5X,I4,1X,F10.2,15X,F15.5,5F8.5/(50X,5F8.5))                MAIN0329
 420 FORMAT (20X,70HNUMBER OF CHEMICAL SPECIES ARE NOT WITHIN LIMITS OFMAIN0330
     1 PROGRAM DIMENSION.)                                              MAIN0331
 425 FORMAT (20X,32HDATA INPUT MAY CONTAIN ERROR(S).,39HCAREFULLY CHECKMAIN0332
     1 PRINTOUT OF INPUT DATA./20X,38HDATA CARDS MAY NOT BE IN PROPER ORMAIN0333
     2DER./5X,19HPROGRAM TERMINATED.)                                   MAIN0334
 430 FORMAT (20X,60HNUMBER OF STAGES ARE NOT WITHIN LIMITS OF PROGRAM DMAIN0335
     1IMENSION.)                                                        MAIN0336
 435 FORMAT (20X,29HFEED MOLE FRACTIONS FOR STAGE,I4,20H DO NOT SUM TO MAIN0337
     11.000)                                                            MAIN0338
 440 FORMAT (20X,87HCALCULATIONS ALLOWED TO PROCEED, BUT THEY MAY NOT CMAIN0339
     1ONVERGE OR THEY MAY NOT BE ACCURATE.)                             MAIN0340
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  445 FORMAT (//20X,15HBOTTOMS RATE OF,E15.5,2X,79HLBMOLES/HR IS NEGATIVMAIN0341
     1E. CAREFULLY CHECK FEED, DISTILLATE, AND SIDESTREAM RATES./5X,16HCMAIN0342
     2ASE TERMINATED.)                                                  MAIN0343
  450 FORMAT (20X,46HBUBBLE-POINT TEMPERATURE CALCULATION FOR STAGE,I4,2MAIN0344
     10H DID NOT CONVERGE IN,14,12H ITERATIONS /20X,23HDURING COLUMN ITEMAIN0345
     2RATION,I4,1H./20X,51HCALCULATIONS ALLOWED TO PROCEED USING LAST VAMAIN0346
     3LUE OF,F13.2,2X,6HDEG. F/)                                        MAIN0347
  455 FORMAT (20X,37HCOMPUTED BUBBLE-POINT TEMPERATURE OF ,F10.2,2X,17HDMAIN0348
     1EG. F, FOR STAGE,I4/20X,19HOF COLUMN ITERATION,I4,68H  IS OUTSIDE MAIN0349
     2OF RANGE OF VALIDITY OF PHYSICAL PROPERTY COEFFICIENTS.)          MAIN0350
  460 FORMAT (20X,59HSHOULD REPEAT RUN WITH VALID PHYSICAL PROPERTY COEFMAIN0351
     1FICIENTS/5X,19HPROGRAM TERMINATED.)                               MAIN0352
  465 FORMAT (20X,22HCOMPUTED VAPOR RATE OF,F15.5,10H FOR STAGE,I4,2X,19MAIN0353
     1HOF COLUMN ITERATION,I4,2X,12HIS NEGATIVE.)                       MAIN0354
  470 FORMAT (20X,110HTHIS MAY BE DUE TO TOO LOW A REFLUX RATIO OR IMPROMAIN0355
     1PER DISTILLATE, SIDESTREAM, OR HEAT TRANSFER SPECIFICATIONS,/20X,4MAIN0356
     25HCAUSING IMPOSSIBLE MATERIAL OR HEAT BALANCES./5X,16HCASE TERMINAMAIN0357
     3TED.)                                                             MAIN0358
  475 FORMAT (20X,23HCOMPUTED LIQUID RATE OF,F15.5,10H FOR STAGE,I4,2X,1MAIN0359
     19HOF COLUMN ITERATION,I4,2X,12HIS NEGATIVE.)                      MAIN0360
  480 FORMAT (20X,46HSHOULD REPEAT RUN WITH REVISED SPECIFICATIONS./)   MAIN0361
      END                                                               MAIN0362
```

```
      SUBROUTINE ASUMVT(JP)                                             ASUM0001
      REAL L1                                                           ASUM0002
      DIMENSION JP(20)                                                  ASUM0003
      COMMON/BLOCK1/JS, IC, B, D, R, TB, TD, T(100), NBPI, NCI,         ASUM0004
     1F(100), TF(100), HF(100), XF(20, 100), Y(20, 100), Z(20, 100),    ASUM0005
     2A(100, 101), X(20,100), W(100), U(100), Q(100), V(100),           ASUM0006
     3KCONST(4, 20), HVCNST(3,20), HLCNST(3,20)                         ASUM0007
      JK = JS - 1                                                       ASUM0008
      L1 = D * R                                                        ASUM0009
      V(2) = L1 + D                                                     ASUM0010
      SUM = 0.0                                                         ASUM0011
      DO 15 K = 2,JK                                                    ASUM0012
      IF (JP(K) .EQ. 2) GO TO 5                                         ASUM0013
      SUM = SUM + W(K) - F(K)                                           ASUM0014
      GO TO 10                                                          ASUM0015
    5 SUM = SUM + W(K)                                                  ASUM0016
   10 V(K+1) = V(2) + SUM                                               ASUM0017
   15 CONTINUE                                                          ASUM0018
      TINC = (TB - TD)/JK                                               ASUM0019
      T(1) = TD                                                         ASUM0020
      DO 20 L = 2,JS                                                    ASUM0021
      T(L) = T(L-1) + TINC                                              ASUM0022
   20 CONTINUE                                                          ASUM0023
      RETURN                                                            ASUM0024
      END                                                               ASUM0025
      SUBROUTINE CLEAN                                                  CLEA0001
      COMMON/BLOCK1/JS, IC, B, D, R, TB, TD, T(100), NBPI, NCI,         CLEA0002
     1F(100), TF(100), HF(100), XF(20, 100), Y(20, 100), Z(20, 100),   CLEA0003
     2A(100, 101), X(20,100), W(100), U(100), Q(100), V(100),          CLEA0004
     3KCONST(4, 20), HVCNST(3,20), HLCNST(3,20)                        CLEA0005
      DO 5 I = 1,100                                                    CLEA0006
      TF(I) = 0.0                                                       CLEA0007
      F(I) = 0.0                                                        CLEA0008
      HF(I) = 0.0                                                       CLEA0009
      W(I) = 0.0                                                        CLEA0010
      U(I) = 0.0                                                        CLEA0011
      Q(I) = 0.0                                                        CLEA0012
      V(I) = 0.0                                                        CLEA0013
      T(I) = 0.0                                                        CLEA0014
    5 CONTINUE                                                          CLEA0015
      DO 15 J = 1,100                                                   CLEA0016
      DO 10 I = 1,20                                                    CLEA0017
      XF (I,J) = 0.0                                                    CLEA0018
      X(I,J) = 0.0                                                      CLEA0019
      Y(I,J) = 0.0                                                      CLEA0020
      Z(I,J) = 0.0                                                      CLEA0021
   10 CONTINUE                                                          CLEA0022
   15 CONTINUE                                                          CLEA0023
      RETURN                                                            CLEA0024
      END                                                               CLEA0025
```

```
      FUNCTION EQUILK (TT,I)                                            EQUI0001
      REAL KCONST                                                       EQUI0002
      COMMON/BLOCK1/JS, IC, B, D, R, TB, TD, T(100), NBPI, NCI,         EQUI0003
     1F(100), TF(100), HF(100), XF(20, 100), Y(20, 100), Z(20, 100),   EQUI0004
     2A(100, 101), X(20,100), W(100), U(100), Q(100), V(100),          EQUI0005
     3KCONST(4, 20), HVCNST(3,20), HLCNST(3,20)                        EQUI0006
      EQUILK = KCONST(1,I) + KCONST(2,I) * TT + KCONST(3,I) * TT * TT   EQUI0007
     1 + KCONST(4,I) * TT * TT * TT                                    EQUI0008
      RETURN                                                            EQUI0009
      END                                                               EQUI0010
      FUNCTION FEEDH (KPHASE, JF)
      COMMON/BLOCK1/JS, IC, B, D, R, TB, TD, T(100), NBPI, NCI,
     1F(100), TF(100), HF(100), XF(20, 100), Y(20, 100), Z(20, 100),
     2A(100, 101), X(20,100), W(100), U(100), Q(100), V(100),
     3KCONST(4, 20), HVCNST(3,20), HLCNST(3,20)
      IF (KPHASE .EQ. 1) GO TO 10
      FEEDH = 0.0
      DO 5 I1 = 1, IC
      FEEDH = FEEDH + XF(I1,JF) * (HLCNST(1,I1) + HLCNST(2,I1)*TF(JF)
     1+ HLCNST(3,I1) * TF(JF)*TF(JF))
    5 CONTINUE
      RETURN
   10 FEEDH = 0.0
      DO 15 I1 = 1,IC
      FEEDH = FEEDH + XF(I1,JF) * (HVCNST(1,I1) + HVCNST(2,I1) * TF(JF)
     1+HVCNST(3,I1) * TF(JF) * TF(JF))
   15 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE FUNC(F1, F2, F3, T1, I, J, EQUILK)
      DIMENSION T1(15)
      COMMON/BLOCK1/JS, IC, B, D, R, TB, TD, T(100), NBPI, NCI,
     1F(100), TF(100), HF(100), XF(20, 100), Y(20, 100), Z(20, 100),
     2A(100, 101), X(20,100), W(100), U(100), Q(100), V(100),
     3KCONST(4, 20), HVCNST(3,20), HLCNST(3,20)
      TEMP1 = 0.0
      TEMP2 = 0.0
      TEMP3 = 0.0
      T2 = T1(I -2)
      T3 = T1(I - 1)
      T4 = T1(I)
      DO 5 I1 = 1, IC
      TEMP1 = TEMP1 + EQUILK (T2,I1) * Z(I1,J)
      TEMP2 = TEMP2 + EQUILK (T3,I1) * Z(I1,J)
      TEMP3 = TEMP3 + EQUILK(T4,I1) * Z(I1,J)
    5 CONTINUE
      F1 = TEMP1 - 1.0
      F2 = TEMP2 - 1.0
      F3 = TEMP3 - 1.0
      RETURN
      END
      SUBROUTINE HEAT (J1, EQUILK)                                      HEAT0001
      COMMON/BLOCK1/JS, IC, B, D, R, TB, TD, T(100), NBPI, NCI,         HEAT0002
     1F(100), TF(100), HF(100), XF(20, 100), Y(20, 100), Z(20, 100),    HEAT0003
     2A(100, 101), X(20,100), W(100), U(100), Q(100), V(100),           HEAT0004
     3KCONST(4, 20), HVCNST(3,20), HLCNST(3,20)                         HEAT0005
      COMMON/BLOCK2/ HV(100), HL(100)                                   HEAT0006
      HV(J1) = 0.0                                                      HEAT0007
      HL(J1) = 0.0                                                      HEAT0008
      T1 = T(J1)                                                        HEAT0009
      DO 5 I1 = 1,IC                                                    HEAT0010
      Y(I1,J1) = EQUILK (T1, I1) * Z(I1, J1)                            HEAT0011
      HV(J1) = HV(J1) + Y(I1,J1) * (HVCNST(1,I1) + HVCNST(2,I1) * T(J1) HEAT0012
     1 + HVCNST(3,I1) * T(J1) * T(J1))                                  HEAT0013
      HL(J1) = HL(J1) + Z(I1,J1) * (HLCNST(1,I1) + HLCNST(2,I1) * T(J1) HEAT0014
     1 + HLCNST(3,I1) * T(J1) * T(J1))                                  HEAT0015
    5 CONTINUE                                                          HEAT0016
      RETURN                                                            HEAT0017
      END                                                               HEAT0018
```

```
      SUBROUTINE QDUTY (QB, QD)                                         QDUT0001
      REAL L                                                            QDUT0002
      DIMENSION L(100)                                                  QDUT0003
      COMMON/BLOCK1/JS, IC, B, D, R, TB, TD, T(100), NBPI, NCI,         QDUT0004
     1F(100), TF(100), HF(100), XF(20, 100), Y(20, 100), Z(20, 100),    QDUT0005
     2A(100, 101), X(20,100), W(100), U(100), Q(100), V(100),           QDUT0006
     3KCONST(4, 20), HVCNST(3,20), HLCNST(3,20)                         QDUT0007
      COMMON/BLOCK2/ HV(100), HL(100)                                   QDUT0008
      L(1) = D * R                                                      QDUT0009
      U(1) = D - V(1)                                                   QDUT0010
      SUM = 0.0                                                         QDUT0011
      JMINS = JS - 1                                                    QDUT0012
      DO 5 K = 2, JMINS                                                 QDUT0013
      SUM = SUM + F(K) - W(K) - U(K)                                    QDUT0014
    5 CONTINUE                                                          QDUT0015
      L(JS - 1) = V(JS) + SUM - D                                       QDUT0016
      QB = L(JS-1) * HL(JS-1) - V(JS) * HV(JS) - B * HL(JS)             QDUT0017
      QD = V(2) * HV(2) - L(1) * HL(1) - V(1) * HV(1) - U(1) * HL(1)    QDUT0018
      RETURN                                                            QDUT0019
      END                                                               QDUT0020
      SUBROUTINE SETUP(I, EQUILK)
      COMMON/BLOCK1/JS, IC, B, D, R, TB, TD, T(100), NBPI, NCI,
     1F(100), TF(100), HF(100), XF(20, 100), Y(20, 100), Z(20, 100),
     2A(100, 101), X(20,100), W(100), U(100), Q(100), V(100),
     3KCONST(4, 20), HVCNST(3,20), HLCNST(3,20)
      M1 = JS + 1
      DO 10 I1 = 1, 100
      DO 5 J = 1,101
      A(I1,J) = 0.0
    5 CONTINUE
C-----1ST ROW (CONDENSER) COEFFICIENTS
   10 CONTINUE
      T1 = T(1)
      A(1,1) = -V(1) * EQUILK(T1,I) - (V(2) - V(1))
      T2 = T(2)
      A(1,2) = V(2) * EQUILK(T2, I)
C-----NTH ROW (REBOILER) COEFFICIENTS
      A(JS,JS-1) = V(JS) + B
      TT = T(JS)
      A(JS,JS) = -V(JS) * EQUILK(TT, I) - B
C-----MIDDLE ROWS (TRAY) COEFFICIENTS
      JMINS = JS - 1
      NSTEP = 0
      DO 20 J1 = 2, JMINS
      SUM = 0.0
      DO 15 K1 = 2, J1
      SUM = SUM + F(K1) - W(K1) - U(K1)
   15 CONTINUE
      A(J1, NSTEP + 1) = V(J1) + SUM - F(J1) + W(J1) + U(J1) - D
      TJ1 = T(J1)
      A(J1, NSTEP + 2) = -((V(J1) + W(J1)) * EQUILK(TJ1, I) + V(J1 + 1)
     1 + SUM - D + U(J1))
      TJ1P = T(J1 + 1)
      A(J1, NSTEP + 3) = V(J1 + 1) * EQUILK(TJ1P, I)
      A(J1, M1) = -F(J1) * XF(I,J1)
      NSTEP = NSTEP + 1
   20 CONTINUE
      RETURN
      END
      FUNCTION TEMPNU(TVAL, J, FLAG)                                    TEMP0001
      INTEGER FLAG                                                      TEMP0002
      EXTERNAL EQUILK                                                   TEMP0003
      DIMENSION XT(15)                                                  TEMP0004
      COMMON/BLOCK1/JS, IC, B, D, R, TB, TD, T(100), NBPI, NCI,         TEMP0005
     1F(100), TF(100), HF(100), XF(20, 100), Y(20, 100), Z(20, 100),    TEMP0006
     2A(100, 101), X(20,100), W(100), U(100), Q(100), V(100),           TEMP0007
     3KCONST(4, 20), HVCNST(3,20), HLCNST(3,20)                         TEMP0008
      FLAG = 0                                                          TEMP0009
      I = 3                                                             TEMP0010
      XT(I-2) = 0.80 * (TVAL + 460.) - 460.                             TEMP0011
      XT(I-1) = 1.20 * (TVAL + 460.) - 460.                             TEMP0012
      XT(I) = TVAL                                                      TEMP0013
    5 DIFF = XT(I) - XT(I - 1)                                          TEMP0014
      STEP = DIFF/(XT(I-1) - XT(I-2))                                   TEMP0015
      DELTA = 1.0 + STEP                                                TEMP0016
      CALL FUNC (F1, F2, F3, XT, I, J, EQUILK)                          TEMP0017
      G = F1 * STEP * STEP - F2 * DELTA * DELTA + F3 * (STEP + DELTA)   TEMP0018
      D1 = G*G - 4.0*F3*STEP*DELTA*(F1*STEP - F2*DELTA + F3)            TEMP0019
C-----TEST FOR QUADRATIC SOLUTION SIGN TO GIVE MAXIMUM DENOMINATOR      TEMP0020
      IF (G .GE. 0.0) GO TO 10                                          TEMP0021
      STEP = -2.0 * F3 * DELTA/(G - SQRT(ABS(D1)))                      TEMP0022
      GO TO 15                                                          TEMP0023
   10 STEP = -2.0 * F3 * DELTA/(G + SQRT(ABS(D1)))                      TEMP0024
   15 I = I + 1                                                         TEMP0025
      XT(I) = XT(I-1) + DIFF * STEP                                     TEMP0026
      IF (ABS((XT(I) - XT(I-1))/XT(I)) .LT. 0.0001) GO TO 25            TEMP0027
      IF ( I .EQ. NBPI) FLAG = 1                                        TEMP0028
      IF (I.EQ.NBPI) GO TO 25                                           TEMP0029
      COMP = ABS(XT(I) -XT(I-3))                                        TEMP0030
      COMP1 = ABS(XT(I) - XT(I - 1))                                    TEMP0031
      COMP2 = ABS(XT(I) - XT(I - 2))                                    TEMP0032
      IF (COMP2 .GT. COMP1) GO TO 20                                    TEMP0033
      IF (COMP .LT. COMP1) XT(I-1) = XT(I-3)                            TEMP0034
      GO TO 5                                                           TEMP0035
   20 IF (COMP .LT. COMP2) XT(I-2) = XT(I-3)                            TEMP0036
      GO TO 5                                                           TEMP0037
   25 TEMPNU = XT(I)                                                    TEMP0038
      RETURN                                                            TEMP0039
      END                                                               TEMP0040
      SUBROUTINE TRIDI (I)                                              TRID0001
      DIMENSION P(100), QA(100)                                         TRID0002
      COMMON/BLOCK1/JS, IC, B, D, R, TB, TD, T(100), NBPI, NCI,         TRID0003
     1F(100), TF(100), HF(100), XF(20, 100), Y(20, 100), Z(20, 100),    TRID0004
     2A(100, 101), X(20,100), W(100), U(100), Q(100), V(100),           TRID0005
     3KCONST(4, 20), HVCNST(3,20), HLCNST(3,20)                         TRID0006
      M1 = JS + 1                                                       TRID0007
      P(1) = A(1,2)/A(1,1)                                              TRID0008
      QA(1) = A(1,M1)/A(1,1)                                            TRID0009
      NMIN = JS - 1                                                     TRID0010
      DO 5 J1 = 2, JS                                                   TRID0011
      P(J1) = A(J1,J1 + 1)/(A(J1,J1) - A(J1,J1-1)*P(J1-1))              TRID0012
      QA(J1) = (A(J1,M1) - A(J1,J1-1)*QA(J1-1))/(A(J1,J1) - A(J1,J1-1)* TRID0013
     1P(J1-1))                                                          TRID0014
    5 CONTINUE                                                          TRID0015
      X(I,JS) = QA(JS)                                                  TRID0016
      DO 10 J1 = 1, NMIN                                                TRID0017
      JSUB = NMIN - J1 + 1                                              TRID0018
      X(I,JSUB) = QA(JSUB) - P(JSUB) * X(I,JSUB + 1)                    TRID0019
   10 CONTINUE                                                          TRID0020
      RETURN                                                            TRID0021
      END                                                               TRID0022
```

```
      SUBROUTINE VAPOR( QB, QD, AFLAG, J2, ALIQ)                        VAP00001
      INTEGER AFLAG                                                     VAP00002
      REAL L                                                            VAP00003
      DIMENSION L(100)                                                  VAP00004
      COMMON/BLOCK1/JS, IC, B, D, R, TB, TD, T(100), NBPI, NCI,         VAP00005
     1F(100), TF(100), HF(100), XF(20, 100), Y(20, 100), Z(20, 100),    VAP00006
     2A(100, 101), X(20,100), W(100), U(100), Q(100), V(100),           VAP00007
     3KCONST(4, 20), HVCNST(3,20), HLCNST(3,20)                         VAP00008
      COMMON/BLOCK2/ HV(100), HL(100)                                   VAP00009
      AFLAG = 0                                                         VAP00010
      Q(JS) = QB                                                        VAP00011
      V(2) = D*R  + V(1) + U(1)                                         VAP00012
      SUM1 = 0.0                                                        VAP00013
      JMIN = JS - 1                                                     VAP00014
      DO 5 J1 = 2, JMIN                                                 VAP00015
      SUM2 = SUM1                                                       VAP00016
      SUM1 = SUM1 + F(J1) - W(J1) - U(J1)                               VAP00017
      V(J1 + 1) =((V(J1) + SUM2 - D) * HL(J1 - 1) - (V(J1) + W(J1)) *   VAP00018
     1HV(J1) - (SUM1 + U(J1) - D) * HL(J1) + F(J1) * HF(J1) - Q(J1))/   VAP00019
     2(HL(J1) - HV(J1 + 1))                                             VAP00020
      L(J1) = V(J1 + 1) + SUM1 - D                                      VAP00021
      IF (V(J1+1) .LT. 0.0) GO TO 10                                    VAP00022
      IF (L(J1) .LT. .0) GO TO 15                                       VAP00023
    5 CONTINUE                                                          VAP00024
      RETURN                                                            VAP00025
   10 AFLAG = 1                                                         VAP00026
      J2 = J1 +1                                                        VAP00027
      RETURN                                                            VAP00028
   15 AFLAG = 2                                                         VAP00029
      J2 = J1                                                           VAP00030
      ALIQ = L(J1)                                                      VAP00031
      RETURN                                                            VAP00032
      END                                                               VAP00033
```

Echo Print of Input Data for Sample Problem (card columns as indicated)

```
        10|       20|       30|       40|       50|       60|
         5       50.      350.      250.        25
     .16650E+01    -.15000E-03     .73500E-04    -.30000E-07
     .84000E+00    -.46600E-02     .49400E-04    -.30330E-07
    -.17700E+00     .49500E-02    -.41500E-05     .22000E-07
    -.87900E-01     .17700E-02     .20310E-06     .13100E-07
     .93000E-01    -.15390E-02     .10370E-04    -.15900E-08
     .83100E+04     .13200E+02     .60200E-02
     .11950E+05     .12350E+02     .22100E-01
     .16550E+05     .90100E+01     .37800E-01
     .19200E+05     .29500E+02     .72000E-02
     .22000E+05     .37000E+02     .00000E-00
     .61200E+04     .93500E+01     .15000E-01
     .36200E+04     .40500E+02    -.13200E-01
     .62800E+04     .25000E+02     .46500E-01
     .68400E+04     .38500E+02     .25200E-01
     .79200E+04     .43500E+02     .30200E-01
         1        16         2         1         1         1         3
       7.5      300.      110.       20.         1
         8         2    213.93       50.
       .03       .20       .37       .35       .05
         9         2    213.93       50.
       .03       .20       .37       .35       .05
        13       37.
         3        3.
         3  .200E+06
```

Sample-problem Calculations--Computer Output

```
                         W H E N D I



           MULTICOMPONENT DISTILLATION BY WANG_HENKE METHOD



      MAXIMUM NUMBER OF ITERATIONS FOR BUBBLE-POINT CALCULATIONS =  15

      MAXIMUM NUMBER OF COLUMN ITERATIONS =   25

      CONSTANT FOR COLUMN ITERATION CONVERGENCE CRITERION =  .01000
```

```
                     COEFFICIENTS OF POLYNOMIAL PHYSICAL-PROPERTY EQUATIONS

                            PROPERTY = A + B*T + C*T**2. + D*T**3.
                                  WITH T IN DEG. F

                            PRESSURE =  250.000  PSIA

                            VALID TEMPERATURE RANGE =    50.00 TO   350.00  DEG. F

                                                                                  PROPERTY VALUE
                COMPONENT        A            B            C            D          AT   200.00 DEG. F
                ---------   -----------  -----------  -----------  -----------    -----------------

K-VALUES
                    1       .16650+01    -.15000-03   .73500-04    -.30000-07           4.33500
                    2       .84000+00    -.46600-02   .49400-04    -.30330-07           1.64136
                    3      -.17700+00     .49500-02  -.41500-05     .22000-07            .82300
                    4      -.87900-01     .17700-02   .20310-06     .13100-07            .37902
                    5       .93000-01    -.15390-02   .10370-04    -.15900-08            .18728
VAPOR ENTHALPIES
(BTU/LBMOLE).
                    1       .83100+04     .13200+02   .60200-02                     11190.79993
                    2       .11950+05     .12350+02   .22100-01                     15303.99988
                    3       .16550+05     .90100+01   .37800-01                     19863.99976
                    4       .19200+05     .29500+02   .72000-02                     25387.99976
                    5       .22000+05     .37000+02   .00000                        29400.00000
LIQUID ENTHALPIES
(BTU/LBMOLE)
                    1       .61200+04     .93500+01   .15000-01                      8590.00000
                    2       .36200+04     .40500+02  -.13200-01                     11192.00012
                    3       .62800+04     .25000+02   .46500-01                     13139.99988
                    4       .68400+04     .38500+02   .25200-01                     15547.99988
                    5       .79200+04     .43500+02   .30200-01                     17827.99976
                CASE NUMBER        1

         NO. OF CHEMICAL COMPONENTS =      5
         NO. OF THEORETICAL STAGES =    16
         NO. OF FEEDS =      2
         NO. OF VAPOR SIDESTREAMS =      1
         NO. OF LIQUID SIDESTREAMS =      1
         NO. OF HEAT-TRANSFER STAGES =      1
         EXTERNAL REFLUX-TO-DISTILLATE MOLE RATIO =          7.50000
         DISTILLATE RATE =        20.00000  LBMOLES/HR  VAP
         ESTIMATED DISTILLATE AND BOTTOMS TEMPERATURES ARE      110.00 AND     300.00 DEG. F

         PARTIAL REBOILER COUNTS AS A STAGE.
         CONDENSER IS NUMBERED AS A STAGE EVEN IF DISTILLATE IS LIQUID.
         STAGES ARE NUMBERED DOWN FROM THE TOP.



                  FEED, SIDESTREAM, AND HEAT-TRANSFER RATE SPECIFICATIONS

                                                  HEAT-TRANSFER
                 FLOW RATE     PHASE     TEMP.        RATE
       STAGE   (LBMOLES/HR)  CONDITION  (DEG. F)    (BTU/HR)      COMPONENT MOLE FRACTIONS FOR COMPONENTS 1 TO  5
       -----   ------------  ---------  --------  ------------    -----------------------------------------------

FEEDS

         8       50.00000      LIQ       213.93                    .03000    .20000    .37000    .35000    .05000
         9       50.00000      LIQ       213.93                    .03000    .20000    .37000    .35000    .05000

SIDESTREAMS

        13       37.00000      VAP
         3        3.00000      LIQ

HEAT TRANSFER,
(-) IF TO STAGE,
(+) IF FROM STAGE

         3                                         .20000+06
```

```
                              STAGE TEMPERATURES AND VAPOR FLOW RATES

                                USED TO INITIALIZE COLUMN ITERATIONS

                                     TEMPERATURE              VAPOR RATE
                           STAGE       (DEG. F)              (LBMOLES/HR)
                           -----     -----------             ------------

                             1          110.00                 20.00000
                             2          122.67                170.00000
                             3          135.33                170.00000
                             4          148.00                170.00000
                             5          160.67                170.00000
                             6          173.33                170.00000
                             7          186.00                170.00000
                             8          198.67                170.00000
                             9          211.33                170.00000
                            10          224.00                170.00000
                            11          236.67                170.00000
                            12          249.33                170.00000
                            13          262.00                170.00000
                            14          274.67                207.00000
                            15          287.33                207.00000
                            16          300.00                207.00000
INTERMEDIATE RESULTS WILL BE PRINTED OUT EVERY    3  COLUMN ITERATIONS

          AFTER ITERATION     1  CALCULATIONS ARE NOT CONVERGED.
          COLUMN ITERATION CONVERGENCE FACTOR IS       .27801+03  , WHICH IS GREATER THAN TOLERANCE OF    .16000

          AFTER ITERATION     2  CALCULATIONS ARE NOT CONVERGED.
          COLUMN ITERATION CONVERGENCE FACTOR IS       .28823+02  , WHICH IS GREATER THAN TOLERANCE OF    .16000
```

```
                              INTERMEDIATE RESULTS FOR ITERATION   3

        TEMP.     VAPOR RATE     LIQUID RATE     LIQUID, FOLLOWED BY VAPOR,MOLE FRACTIONS            LIQUID MOLE
STAGE  (DEG. F)  (LBMOLES/HR)   (LBMOLES/HR)      COMPONENTS 1 TO  5                                 FRACTION SUM
-----  --------  ------------   ------------    ------------------------------------------------    ------------
  1     116.41      20.00000      150.00000     .05713     .86081     .03457     .00003     .00000

                                                                                                       .95255
                                                .15571     .83058     .01371     .00000     .00000
  2     129.15     170.00000      151.82304     .02425     .85864     .07324     .00015     .00000

                                                                                                       .95629
                                                .07119     .89505     .03374     .00003     .00000
  3     137.86     171.82304      180.96527     .01312     .81019     .13825     .00070     .00000

                                                                                                       .96226
                                                .04039     .88991     .06956     .00014     .00000
  4     147.77     203.96527      174.49607     .00842     .72098     .23892     .00291     .00001

                                                                                                       .97124
                                                .02731     .84047     .13156     .00066     .00000
  5     159.66     197.49607      166.39819     .00672     .59965     .36532     .01042     .00011

                                                                                                       .98222
                                                .02322     .75202     .22207     .00269     .00001
  6     173.65     189.39819      157.60826     .00593     .46392     .49057     .03181     .00078

                                                                                                       .99300
                                                .02208     .63611     .33229     .00942     .00010
  7     189.73     180.60826      147.82842     .00539     .33529     .57386     .08197     .00426

                                                                                                      1.00077
                                                .02194     .51159     .43754     .02823     .00070
  8     208.90     170.82842      196.36891     .00490     .22935     .57645     .17501     .01789

                                                                                                      1.00360
                                                .02230     .39897     .50347     .07152     .00374
  9     221.93     169.36891      251.56181     .00297     .16615     .59229     .21903     .02465

                                                                                                      1.00509
                                                .01456     .31530     .56431     .09983     .00600
 10     231.94     174.56181      255.14892     .00083     .11329     .63553     .23271     .02511

                                                                                                      1.00746
                                                .00427     .22919     .64491     .11480     .00683
 11     241.07     178.14892      257.19673     .00021     .07082     .65553     .25702     .02610

                                                                                                      1.00969
                                                .00116     .15169     .70336     .13597     .00782
 12     250.52     180.19673      256.85065     .00005     .03990     .64187     .30140     .02847

                                                                                                      1.01168
                                                .00029     .09055     .72870     .17108     .00938
 13     262.11     179.85065      253.65458     .00001     .01914     .58227     .37776     .03442

                                                                                                      1.01360

                                                .00006     .04656     .70744     .23326     .01268
 14     275.33     213.65458      249.26080     .00000     .00845     .48612     .47404     .04667

                                                                                                      1.01529
                                                .00001     .02222     .63702     .32134     .01941
 15     290.52     209.26080      245.62087     .00000     .00339     .36751     .57534     .07057

                                                                                                      1.01681
                                                .00000     .00970     .52417     .43267     .03346
 16     306.86     205.62087       40.00000     .00000     .00120     .24678     .65703     .11317

                                                                                                      1.01817
                                                .00000     .00375     .38462     .55036     .06127
                AFTER ITERATION    3  CALCULATIONS ARE NOT CONVERGED.
                COLUMN ITERATION CONVERGENCE FACTOR IS      .19458+02  , WHICH IS GREATER THAN TOLERANCE OF     .16000

                AFTER ITERATION    4  CALCULATIONS ARE NOT CONVERGED.
                COLUMN ITERATION CONVERGENCE FACTOR IS      .14442+02  , WHICH IS GREATER THAN TOLERANCE OF     .16000

                AFTER ITERATION    5  CALCULATIONS ARE NOT CONVERGED.
                COLUMN ITERATION CONVERGENCE FACTOR IS      .10768+02  , WHICH IS GREATER THAN TOLERANCE OF     .16000
```

(Intermediate results between column iterations 5 and 18 are not shown here.)

```
AFTER ITERATION   18  CALCULATIONS ARE NOT CONVERGED.
COLUMN ITERATION CONVERGENCE FACTOR IS      .19422+00  , WHICH IS GREATER THAN TOLERANCE OF    .16000

AFTER ITERATION   19  CALCULATIONS ARE CONVERGED.
COLUMN ITERATION FACTOR IS    .14041    WHICH IS LESS THAN TOLERANCE OF    .16000
FINAL DETAILED RESULTS WILL NOW BE PRINTED.
```

```
                                          FINAL RESULTS

                               PRODUCT STREAMS AND EXCHANGER DUTIES

             FROM   PHASE     TEMP.      FLOW RATE       COMPONENT MOLE FRACTIONS
  STREAM    STAGE CONDITION (DEG. F)   (LBMOLES/HR)      FOR COMPONENTS 1 TO   5
  ------    ----- --------- --------   ------------   --------------------------------------------------

DISTILLATE    1      VAP     120.04        20.00000     .14869     .82518     .02611     .00001     .00000

SIDESTREAM   13      VAP     263.95        37.00000     .00005     .03411     .71145     .24127     .01310

SIDESTREAM    3      LIQ     145.19         3.00000     .01217     .75605     .22819     .00126     .00000

 BOTTOMS     16      LIQ     307.84        40.00000     .00000     .00083     .23616     .65151     .11287

               CONDENSER DUTY =        .86482+06  BTU/HR
               REBOILER DUTY =        -.16103+07  BTU/HR
```

```
                                              FINAL RESULTS

                                           INTERNAL CONDITIONS

                     FLOWS FROM STAGES
        TEMP.     VAPOR RATE     LIQUID RATE   LIQUID MOLE FRACTIONS                      VAPOR MOLE FRACTIONS
STAGE  (DEG. F)  (LBMOLES/HR)   (LBMOLES/HR)   COMPONENTS 1 TO    5                       COMPONENTS 1 TO    5
-----  ---------  ------------  ------------  ------------------------------------------  ----------------------------------------

  1     120.04                   150.00000   .05581  .87461  .06579  .00006  .00000
  2     134.28    170.00000                                                           .06692  .87167  .06136  .00006  .00000
  2     134.28                   150.29145   .02302  .84233  .13122  .00030  .00000
  3     145.19    170.26730                                                           .03783  .84262  .11928  .00027  .00000
  3     145.19                   177.23235   .01217  .75605  .22819  .00126  .00000
  4     157.34    200.17688                                                           .02581  .76449  .20857  .00113  .00000
  4     157.34                   170.30442   .00771  .63015  .35619  .00459  .00002
  5     170.55    193.25089                                                           .02233  .65296  .32061  .00408  .00002
  5     170.55                   163.21043   .00615  .49016  .48884  .01431  .00017
  6     184.37    186.18095                                                           .02151  .53047  .43530  .01258  .00015
  6     184.37                   156.47856   .00545  .36098  .59450  .03842  .00100
  7     198.83    179.48260                                                           .02146  .41901  .52514  .03353  .00087
  7     198.83                   148.93611   .00499  .25756  .64395  .08947  .00471
  8     215.31    171.96900                                                           .02175  .33186  .56477  .07753  .00408
  8     215.31                   199.35038   .00459  .18205  .61695  .17902  .01804
  9     226.97    172.40632                                                           .01400  .26101  .61310  .10553  .00636
  9     226.97                   255.76256   .00276  .13241  .61975  .22118  .02456
 10     236.25    178.83308                                                           .00394  .18211  .68615  .12063  .00716
 10     236.25                   259.79888   .00074  .08694  .65343  .23473  .02496
 11     244.43    182.87306                                                           .00104  .11639  .73237  .14207  .00812
 11     244.43                   261.64505   .00019  .05273  .66264  .25941  .02596
 12     253.01    184.71458                                                           .00025  .06764  .74449  .17792  .00970
 12     253.01                   260.74068   .00004  .02903  .63912  .30440  .02842
 13     263.95    183.80822                                                           .00005  .03411  .71145  .24127  .01310
 13     263.95                   256.95607   .00001  .01369  .57210  .38079  .03452
 14     276.82    217.00411                                                           .00001  .01605  .63336  .33053  .02005
 14     276.82                   252.24998   .00000  .00597  .47253  .47578  .04691
 15     291.77    212.29745                                                           .00000  .00693  .51647  .44215  .03444
 15     291.77                   248.55315   .00000  .00237  .35410  .57405  .07077
 16     307.84    208.60081                                                           .00000  .00266  .37623  .55848  .06262
```

Comments on Sample-problem Results

For this fairly complicated problem, involving two feeds, two sidestreams, and a heat-transfer stage, convergence of the column iterations was not rapid. A total of 19 column iterations was required before the convergence factor, STD, decreased to a value less than the convergence criterion, T0L. An execution time of 5.6 seconds was required to solve the problem on a Univac 1108 using Exec 8. This is equivalent to 0.3 second per column iteration.

The liquid sidestream from stage 3 contains 75.6 mole percent propane, while the vapor sidestream from stage 13 contains 71.1 mole percent n-butane. The internal conditions indicate that a sidestream richer in n-butane could probably have been obtained from stage 12. The intercooler on stage 3 produces an additional 27 lbmoles/hr of reflux at a temperature of 145°F. Essentially no n-hexane appears in the distillate, and no ethane appears in the bottoms. An interesting student exercise is to plot the temperature, vapor/liquid traffic, and composition against stage number, using the final results. Alternatively, the student could alter the program to call a subprogram to make such plots.

Multicomponent Stripping and Absorption

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Technical Description

Two classical approaches to the solution of multicomponent stage-by-stage stripping or absorption calculations have been popular. In the first method, the number of required theoretical stages is determined for a specified recovery of one key component and a stripping-vapor rate or an absorbing-liquid rate greater than the minimum. In the second method, the number of theoretical stages and the stripping-vapor rate or absorbing-liquid rate are specified; and the split of each component is computed. Both methods involve tedious iterative calculations. Thus, much effort has been expended in writing digital-computer programs for making the computations. In general, stripping and absorption calculations are more difficult to converge than distillation calculations;[1] and the second method, which is basically a Thiele-Geddes[2] approach, has been more successfully programmed. STAB is a program for making method-two/type calculations by use of a matrix formulation originally applied by Amundson and Pontinen[3] and further extended and refined by Wang and Henke.[4] Rigorous material and energy balances are made around each theoretical stage. The sum-rate technique described by Sujata[5] and more recently by Burningham and Otto[6] is utilized to compute stage temperatures. This technique avoids the unreliable temperature calculations that may result from the use of the bubble-point technique, as mentioned by Smith.

A typical problem statement follows.[7] A six-theoretical-stage absorber operating at 75 psia is to treat 18,000,000 SCFD (60°F and 1 atm) of a gas containing:

---

[1] B. D. Smith, *Design of Equilibrium Stage Processes* (New York: McGraw-Hill Book Co., 1963), pp. 462-464.

[2] E. W. Thiele and R. L. Geddes, *Ind. Eng. Chem.*, *25* (1933), 289.

[3] N. R. Amundson and A. J. Pontinen, *Ind Eng. Chem.*, *50* (1958), 730.

[4] J. C. Wang and G. E. Henke, *Hydrocarbon Processing*, *45*, 8 (1966), 155.

[5] A. D. Sujata, *Hydrocarbon Processing and Petroleum Refiner*, *40*, 12 (1961), 137.

[6] D. W. Burningham and F. D. Otto, *Hydrocarbon Processing*, *46*, 10 (1967), 163.

[7] The solution to this problem is given below in the section entitled "Sample Problem."

Compound	Mole %
methane	83.0
ethane	8.4
propane	4.8
n-butane	2.6
n-pentane	1.2
	100.0

The tower will be supplied with 300,000 gal/day of an absorber oil of 40° API gravity and 161 average molecular weight. The inlet-gas and oil temperatures are 60°F and 90°F, respectively. The products are to be calculated, as are the column interior temperatures, the vapor/liquid traffic, and the vapor/liquid compositions for each theoretical stage.

The mathematical formulation based on a theoretical stage model is shown in Figure 1. Each stage can accept up to one feed stream and can produce up to one vapor sidestream and up to one liquid sidestream. Heat may be transferred to or from a stage. The governing equations for each stage, as given by Burningham and Otto, consist of:

1. overall material balances,
2. component material balances,
3. component equilibrium relationships in terms of K values,
4. mole-fraction sums (vapor or liquid),
5. heat balances.

Thus, for each stage, with the feed (if any) completely specified, with the heat-transfer rate (if any) specified, and with vapor- and/or liquid-sidestream total flow rates (if any) specified, there exist 3 + 2C equations, where C equals the number of chemical species, in 3 + 2C unknowns; namely,

$x_{i,j}$ = equilibrium liquid mole fractions,

$y_{i,j}$ = equilibrium vapor mole fractions,

L_j = liquid flow rate from one stage to an adjacent stage,

V_j = vapor flow rate from one stage to an adjacent stage,

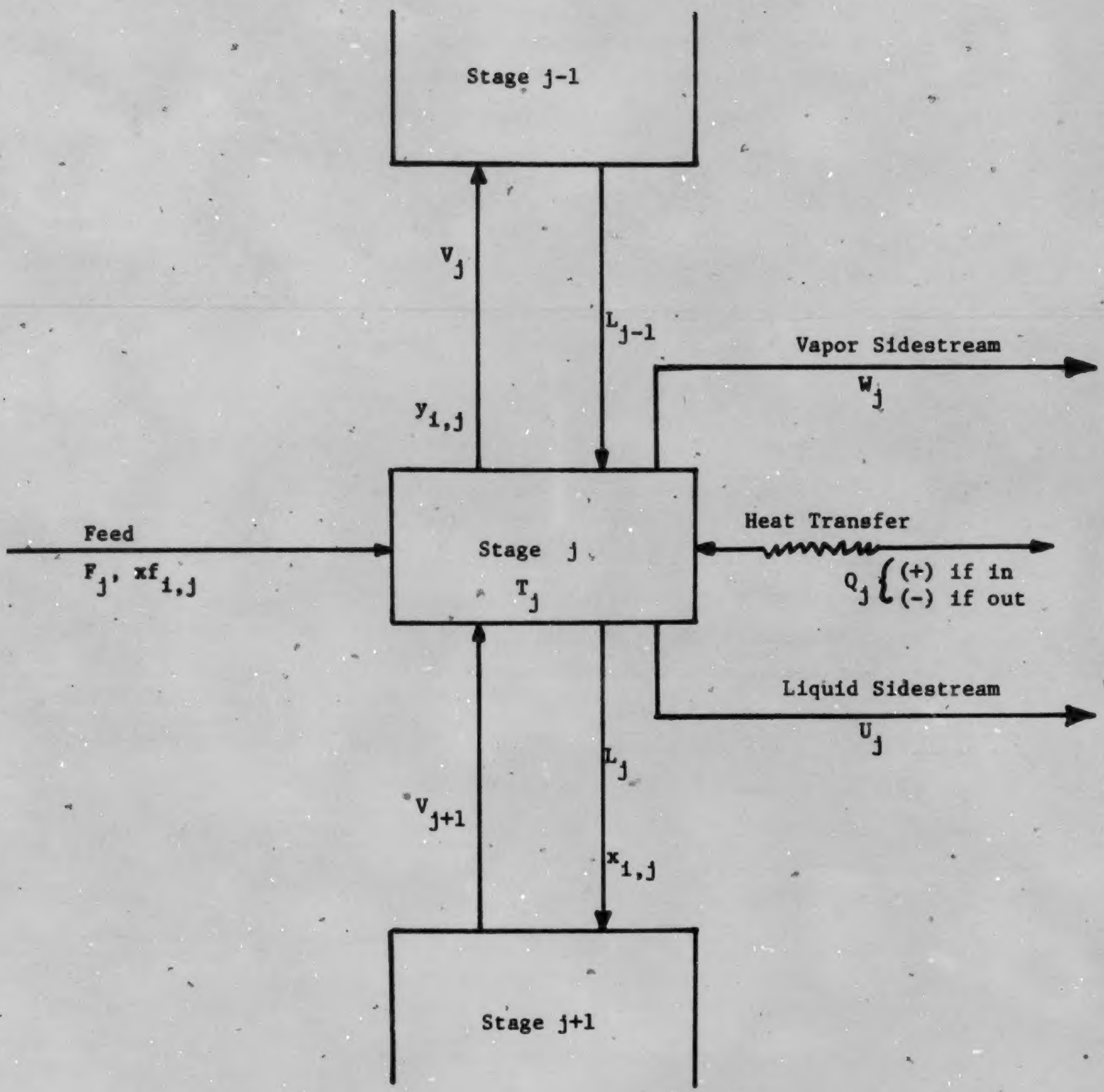
Stage j-1
V_j
L_{j-1}
Vapor Sidestream
W_j
$y_{i,j}$
Feed
F_j, $xf_{i,j}$
Stage j
T_j
Heat Transfer
Q_j { (+) if in (-) if out
Liquid Sidestream
U_j
L_j
V_{j+1}
$x_{i,j}$
Stage j+1

FIGURE 1. THEORETICAL STAGE MODEL
(Nomenclature is that of Wang-Henke rather than Burningham-Otto)

and

T_j = stage equilibrium temperature,

where i refers to the chemical species, i = 1 to C, and j refers to the stage number, j = 1 to N.

By combining the first three types of governing equations listed above, a set of C nonlinear algebraic matrix equations is obtained. The equations are linearized by use of assumed values of V_j and T_j and then solved for the liquid-phase mole fractions, $x_{i,j}$, by means of a modified Gauss elimination scheme that overcomes the dificiencies of some previous methods in that it does not produce small values from differences between large numbers nor does it produce negative mole fractions. The sum-rates technique is then applied to compute a new set of liquid and vapor rates by use of the relationships,

$$\left(L_j\right)_{new} = \left(L_j\right)_{old} \sum_{i=1}^{C} x_{i,j}$$

and

$$\left(V_j\right)_{new} = \left(L_{j-1}\right)_{new} - \left(L_j\right)_{new} + \sum_{k=j}^{N} \left(F_k - U_k - W_k\right).$$

A new set of stage temperatures, T_j, is obtained from the heat-balance equations by means of the Newton-Raphson method.[8]

The entire calculational procedure for the distillation column is repeated until the differences between successive sets of computed stage temperatures satisfy the overall convergence criterion,

$$\sum_{j=1}^{N} \left(\Delta T_j\right)^2 \leq 0.01\ N.$$

The somewhat arbitrary value of 0.01 may be changed if desired. The assumed values of V_j and T_j for each column iteration after the first one are the calculated values from the previous iteration (successive substitution technique). To initiate the first column iteration, a linear temperature profile is assumed on the basis of estimates of the overhead and bottoms temperatures; and vapor rates are calculated on the basis of the assumption of constant molal overflow.

---

[8] F. B. Hildebrand, *Introduction to Numerical Analysis* (New York: McGraw-Hill Book Co., 1956), pp. 443-451.

In general, STAB converges to a successful solution unless the specifications result in zero or negative vapor/liquid traffic or unless stage temperatures correspond to values outside the range of validity of the physical-property correlations utilized. The K values are computed for each chemical species from a cubic polynomial in the temperature:

$$K_{i,j} = \alpha_i + \beta_i T_j + \gamma_i T_j^2 + \delta_i T_j^3. \tag{1}$$

The liquid and vapor enthalpy values for each stream are computed from:

$$h = \sum_{i=1}^{C} h_i x_i, \tag{2}$$

where

$$h_i = a_i + b_i T + c_i T^2, \tag{3}$$

and from

$$H = \sum H_i y_i, \tag{4}$$

where

$$H_i = A_i + B_i T + C_i T^2. \tag{5}$$

Values of the coefficients in Equations 1, 3, and 5 must be supplied by the user for the particular chemical species and the column operating pressure.

Numerous examples of absorption and stripping calculations exist in the literature. Many of the general sources are referenced by King,[9] who also presents an excellent discussion on convergence problems associated with absorption and stripping operations. Hardy *et al.*[10] present a number of worthwhile examples; however, the physical-property correlations utilized are not the same as Equations 1, 3, and 5 above. Similar problems can readily be formulated by use of the many physical-property polynomial-equation coefficients of the same form as those employed here, as given by Lyster *et al.*[11,12] For problems in which they are not already available, the physical-property polynomial-equation coefficients may be readily obtained by means of standard curve-fitting techniques[13] by use of analytical, graphical, or tabular physical-property data or correlations.

---

[9] C. J. King, *Separation Processes* (New York: McGraw-Hill Book Co., 1971), pp. 493, 541.

[10] B. W. Hardy *et al.*, *Hydrocarbon Processing and Petroleum Refiner*, *40*, 7 (1961), 237.

In its present form, STAB is restricted to feeds that are either liquid or vapor (not those that are partially vaporized).

Educational Aspects

STAB may be used in any course that covers the principles of multicomponent absorption and/or stripping. For introductory courses, the program can afford the student the opportunity to solve one or more simple problems. Examples can be chosen to illustrate the degree to which deviations can occur from the classical modified Kremser method.[14]

In more advanced equilibrium-stage courses, a variety of more difficult problems may be assigned, involving, for example,

1. the effect of using two absorber oils entering at different stages,
2. the effect of using an intercooler to maintain a low absorption temperature,
3. the effect of using a reheater for stripping vapor.

While the program may be used as is for a variety of problems, it may be desirable to assign problems involving modifications to the program; *e.g.*,

1. addition of a feed flash subroutine to permit applications involving partially vaporized feeds,

---

[11] W. N. Lyster *et al.*, *Petroleum Refiner, 38*, 6 (1959), 221.

[12] *Ibid.*, 10 (1959), 139.

[13] B. Carnahan, H. A. Luther, and J. O. Wilkes, *Applied Numerical Methods* (New York: John Wiley and Sons, Inc., 1969), chap. 1.

[14] M. Souders and G. G. Brown, *Ind. Eng. Chem.*, *24* (1932), 519.

2. addition of a subroutine to accelerate the convergence of the column iterations instead of reliance on successive substitution with respect to V_j and T_j,

3. replacement of the polynomial K-value treatment by a self-contained K-value calculation method, such as the Chao-Seader,[15] Lee-Edmister,[16] or Prausnitz-Chueh[17] methods.

Available textbooks, particularly King's,[18] suggest a number of other possible interesting problems and/or program modifications that might be attempted.

At least three one-hour lectures are required to present the theory of the method, unless the Wang-Henke method for distillation has already been presented; then only one additional hour's lecture is necessary. A further one-hour lecture should be used to discuss the results of the first problem assignment.

Program Description

General Structure, Limitations, and History

STAB consists of a main driver program, seven subroutines, and four function subprograms. The overall communication scheme, the interrelationships among and the purposes of the main driver program and the subprograms, are shown in Figure 2. Besides handling all input and output tasks, the main driver program sets up and checks convergence of the column iterations. Successive cases using the same physical-property constants are automatically attempted until an end-of-file is reached (no more data cards). Eight blocks of labeled common are used.

The chief limitations of the program are:

1. a maximum of 20 chemical components;

---

[15] K. C. Chao and J. D. Seader, *AIChE J.*, *7* (1961), 598.

[16] B. Lee and W. C. Edmister, *AIChE J.*, *17* (1971), 1412.

[17] J. M. Prausnitz and P. L. Chueh, *Computer Calculations for High Pressure Vapor-Liquid Equilibria* (Englewood Cliffs, N. J.: Prentice-Hall, Inc., 1968).

[18] King, *op. cit.*

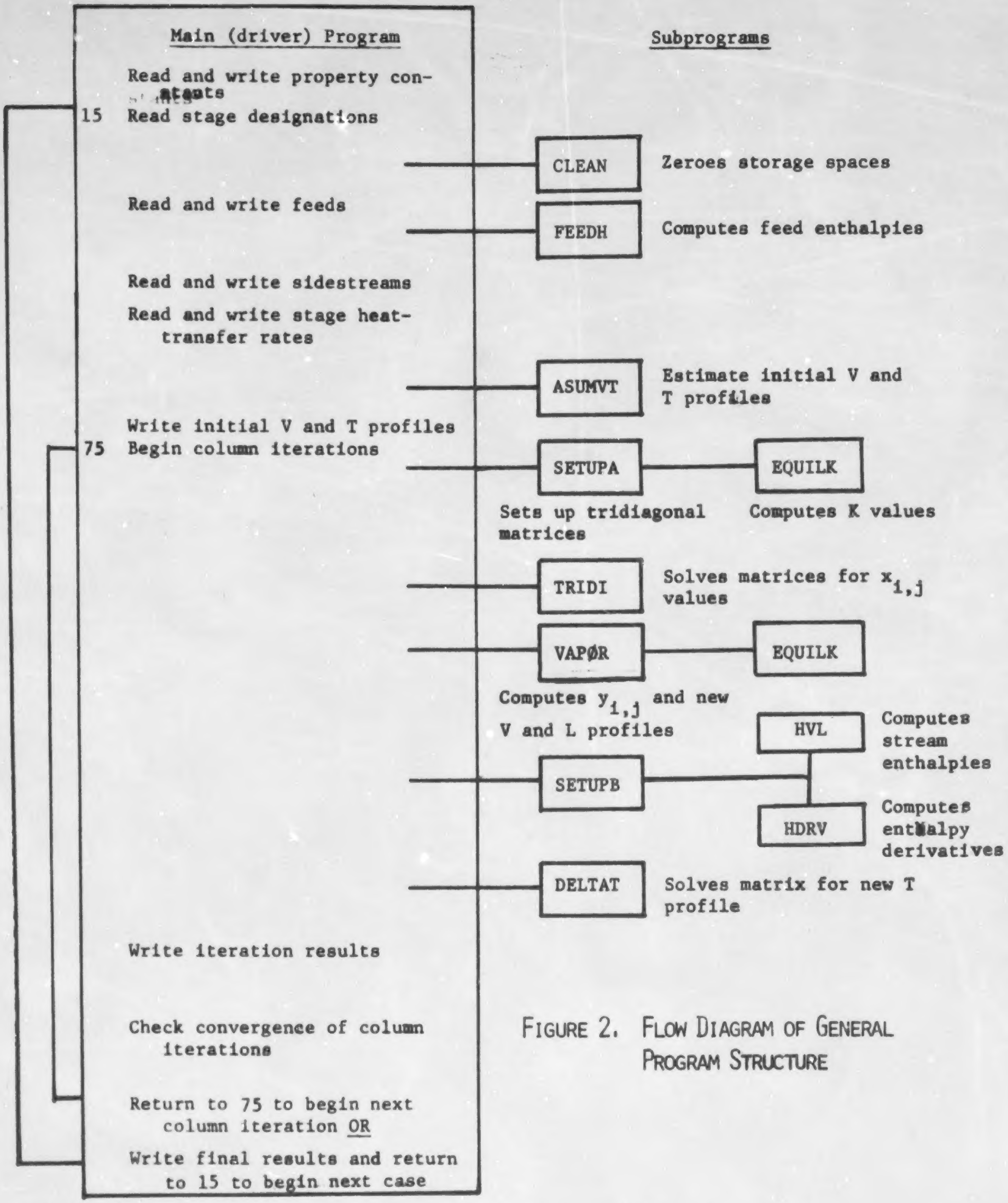
Main (driver) Program
Subprograms
Read and write property constants
15 Read stage designations
CLEAN
Zeroes storage spaces
Read and write feeds
FEEDH
Computes feed enthalpies
Read and write sidestreams
Read and write stage heat-transfer rates
ASUMVT
Estimate initial V and T profiles
Write initial V and T profiles
75 Begin column iterations
SETUPA
EQUILK
Sets up tridiagonal matrices
Computes K values
TRIDI
Solves matrices for $x_{i,j}$ values
VAPØR
EQUILK
Computes $y_{i,j}$ and new V and L profiles
HVL
Computes stream enthalpies
SETUPB
HDRV
Computes enthalpy derivatives
DELTAT
Solves matrix for new T profile
Write iteration results
Check convergence of column iterations
Return to 75 to begin next column iteration OR
Write final results and return to 15 to begin next case

FIGURE 2. FLOW DIAGRAM OF GENERAL PROGRAM STRUCTURE

2. a maximum of 100 equilibrium stages;

3. a maximum of 15 iterations for converging the new temperature-profile calculations (this limit, NHBI, is set in a DATA statement in the main driver program and may be changed if desired); a maximum of NCI column iterations (if NCI is not specified in the input data, a value of 15 is used);

4. single-phase feeds.

The program was written in FØRTRAN IV in 1968 for use on a Univac 1108. It has been used successfully every year since then. The normal system of units employed includes °F, Btu/hr, lbmoles/hr, Btu/lbmole, and psia. Stages are numbered down from the top.

CØMMØN/BLØCK1

Symbol	*Type*	*Description and Usual Symbol*
F	real	Feed rate, F
JS	integer	Total number of theoretical stages, N
T	real	Equilibrium-stage temperature, T
U	real	Liquid-sidestream flow rate, U
V	real	Vapor flow rate leaving a stage to go to an adjacent stage, V
W	real	Vapor-sidestream flow rate, W
XF	real	Feed mole fractions, xf

CØMMØN/AA1

Symbol	*Type*	*Description and Usual Symbol*
HF	real	Feed molal enthalpy
Q	real	Heat-transfer rate to or from a stage, Q
TF	real	Feed temperature

CØMMØN/AA2

Symbol	*Type*	*Description and Usual Symbol*
HLCNST	real	Coefficients of liquid-enthalpy equation
HVCNST	real	Coefficients of vapor-enthalpy equation
IC	integer	Total number of chemical components
L	real	Liquid flow rate leaving a stage to go to an adjacent stage, L

The FØRTRAN symbols for the enthalpy coefficients are related to the usual symbols, given in Equations 3 and 5, as follows:

HLCNST(1,JK) = a_i HVCNST(1,JK) = A_i

HLCNST(2,JK) = b_i HVCNST(2,JK) = B_i

HLCNST(3,JK) = c_i HVCNST(3,JK) = C_i

CØMMØN/AA3

Symbol	*Type*	*Description*
KCØNST	real	Coefficients of polynomial K-value equation
TD	real	Initial estimate of top-stage temperature
TB	real	Initial estimate of bottom-stage temperature

The FØRTRAN symbols for the K-value coefficients are related to the usual symbols, given in Equation 1, as follows:

KCØNST(1,JK) = α_i KCØNST(3,JK) = γ_i

KCØNST(2,JK) = β_i KCØNST(4,JK) = δ_i

CØMMØN/AA4

Symbol	*Type*	*Description and Usual Symbol*
X	real	Liquid-phase mole fractions, x

CØMMØN/AA5

Symbol	*Type*	*Description and Usual Symbol*
Z	real	Normalized liquid-phase mole fractions
ZY	real	Normalized vapor-phase mole fractions
ADDX	real	Sum of liquid-phase mole fractions
Y	real	Vapor-phase mole fractions, y

CØMMØN/BA1

Symbol	*Type*	*Description*
A	real	Coefficients of tridiagonal matrix of component material-balance equations

CØMMØN/BA2

Symbol	*Type*	*Description*
AA	real	Coefficients of tridiagonal matrix of heat-balance equations

The above common-block variables are not repeated in program-variable lists to follow.

Main (Driver) Program

Principal variables:

Symbol	*Type*	*Description and Usual Symbol*
JF	integer	Feed stage number
JP	integer	Feed phase condition (1 = vapor, 2 = liquid)
JQ	integer	Heated or cooled stage number
JSL	integer	Liquid-sidestream stage number
JSV	integer	Vapor-sidestream stage number
K1	integer	Column-iteration number
KP	integer	Frequency of printout for results of column iteration

LUIN	integer	Logical unit number for input device (card reader); preset to 5 in a DATA declaration
LUØUT	integer	Logical unit number for output device (printer); preset to 6 in a DATA declaration
NC	integer	Case number
NCI	integer	Maximum number of column iterations; set at 15 if not specified
NHBI	integer	Maximum number of heat-balance iterations; preset at 15 in a DATA declaration
NØF	integer	Number of feeds
NØLS	integer	Number of liquid sidestreams
NØQS	integer	Number of heated or cooled stages
NØVS	integer	Number of vapor sidestreams
PHASE	integer	Feed-phase condition (1 = vapor, 2 = liquid)
QRATE	real	Heat-transfer rate to a stage [(-) if heated, (+) if cooled], Q
RATE	real	Liquid-sidestream flow rate, U
STD	real	Sum of the square of the differences between successive sets of stage temperatures
SUM	real	Net inflow to an upper section of the column, of feeds and/or sidestreams
SUMFD	real	Sum of feed flow rates
TEMP	real	Feed temperature
TAL	real	Column-iteration-convergence-criterion constant; preset to 0.01 in a DATA declaration
TØL	real	Column-iteration-convergence criterion
TS	real	Stage temperatures used to begin a column iteration
VRATE	real	Vapor-sidestream flow rate, W
XFEED	real	Feed mole fractions, xf
XFLØW	real	Feed flow rate, F

Subprograms called:

Name	*Type*	*Purpose*
CLEAN	Subroutine	Zeroes out TF, F, HF, W, U, Q, and XF arrays
FEEDH	Real Function	Computes feed molal enthalpies
ASUMVT	Subroutine	Calculates initial temperature and vapor profile on the basis of a linear interpolation between TB and TD input values and the assumption of constant molal overflow, respectively

SETUPA	Subroutine	Calculates the coefficients, A, of the tridiagonal matrices that represent the linearized stage equations in terms of the liquid-phase mole fractions
TRIDI	Subroutine	Solves the tridiagonal matrices for the liquid-phase mole fractions by a modified Gauss elimination method
VAP0R	Subroutine	Computes vapor-phase mole fractions from equilibrium equations and new vapor and liquid traffic from sum-rates technique
SETUPB	Subroutine	Calculates the coefficients, AA, of the tridiagonal matrix that represents the stage heat-balance equations
DELTAT	Subroutine	Solves the tridiagonal matrix for the stage-temperature changes and then computes the new stage temperatures

Input (each line corresponds to one card):

Group	*Data Items*	*Format*
1	IC, TL0W, THI, P, NCI[19]	I10,3F10.2,I10
2	KC0NST(1,1), KC0NST(2,1), KC0NST(3,1), KC0NST(4,1)	4E15.5
	KC0NST(1,2), KC0NST(2,2), KC0NST(3,2), KC0NST(4,2)	4E15.5
	. . . .	.
	. . . .	.
	. . . .	.
	KC0NST(1,IC),KC0NST(2,IC),KC0NST(3,IC),KC0NST(4,IC)	.
3	HVCNST(1,1), HVCNST(2,1), HVCNST(3,1)	3E15.5
	HVCNST(1,2), HVCNST(2,2), HVCNST(3,2)	3E15.5
	. . .	.
	. . .	.
	. . .	.
	HVCNST(1,IC), HVCNST(2,IC), HVCNST(3,IC)	.
4	Same as Group 3, only HLCNST instead of HVCNST	

---

[19] If a value of NCI is not specified, a default value of 15 is used.

5	NC, JS, NØF, NØVS, NØLS, NØQS, KP[20]	7I10
6	TB, TD	2F10.2
7	JF, PHASE, TEMP, XFLØW XFEED(1), XFEED(2), ... XFEED(IC)	2I10,2F10.2 5F10.5 . . .
	Repeat Group 7 for other feeds, if any, up to NØF	
8[21]	JSV, VRATE	I10,F10.2
	Repeat Group 8 for other vapor sidestreams, if any, up to NØVS	
9[22]	JSL, RATE	I10,F10.2
	Repeat Group 9 for other liquid sidestreams, if any, up to NØLS	
10[23]	JQ, QRATE	I10,F15.5
	Repeat Group 10 for other stages that are heated or cooled, if any, up to NØQS	

Order of chemical species must be consistent and is usually in descending volatility. Multiple cases may be run using the same components and the same physical-property constants by repeating data-card groups 5 through 10 as many times as desired. All case problems must include at least two feeds; a vapor feed must be sent to the last stage, and a liquid feed must be sent to the first stage.

---

[20] If a value of KP is not specified, a default value of 10 is used.

[21] Delete group if NØVS = 0.

[22] Delete group if NØLS = 0.

[23] Delete group if NØQS = 0.

Output:

All input data and initial T and V profiles are printed. For each column iteration, the convergence factor, STD, is compared with the tolerance factor, TØL. At the conclusion of the final column iteration or when NCI is reached, a product summary and the following interior quantities are printed for each stage: T, V, L, x_i, and y_i. The results from intermediate column iterations may be obtained by setting KP to a value greater than 0 and less than NCI. For example, KP = 2 in the data input will cause the results of iterations 2, 4, 6, etc., to be printed, until convergence is achieved.

Error messages:

A number of error flags and messages are provided in the main program to guide the user in the event that errors are detected. In general, the error messages are self-explanatory and are not described here. The detected errors affect the program in any one of three ways:

1. allow the case to proceed,
2. terminate the case and proceed to the next case,
3. terminate the program.

Input values of the physical-property-correlation coefficients are not tested for possible errors. Instead, values of the component physical properties are computed at the mid-temperature of the valid range and are printed out with the coefficients so that the user can scrutinize them.

The variables defined above are not repeated if they appear in the subprograms discussed below. If a subprogram contains no new principal variables, does not call other subprograms, and contains no complicated algorithms, it is not discussed below.

Subroutine SETUPA

This subroutine computes the coefficients, A, of the tridiagonal matrix for each chemical component at a time. The two-dimensional A array here replaces the one-dimensional A, B, C, and D arrays used in the Burningham-Otto article. Thus, including the constant vector, each component matrix has the dimensions, JS by (JS + 1). The matrix equation is given as Equation 6 in the Burningham-Otto article, with coefficients defined in Equation 7 of that article. The derivation of these equations is a good student exercise in advanced courses.

Principal variables:

Symbol	*Type*	*Description*
JMINS	integer	Number of stages, less one
M1	integer	Number of columns in the matrix
NSTEP	integer	Related to a particular column of the matrix

Subprograms called:

Name	*Type*	*Purpose*
EQUILK	real function	Computes K values at designated temperature for designated chemical species

Subroutine TRIDI

This subroutine solves the tridiagonal matrix for the x_j values for a particular component by a modified Gauss elimination method, described in the Burningham-Otto article on page 169.

Principal variables:

Symbol	*Type*	*Corresponding Symbol in Burningham-Otto Article*
P(1)	real	p_1
QA(1)	real	q_1
P(J1)	real	p_n
QA(J1)	real	q_n

Subroutine VAP0R

This subroutine computes the stage vapor-phase mole fractions from the definition of the K value by use of the liquid-phase mole fractions computed in TRIDI. New liquid- and vapor-rate profiles are then computed by means of the sum-rates technique described above in the "Technical Description" section. The liquid and vapor mole fractions are normalized such that they sum to 1.0 for each stage. The real function, EQUILK, is called.

Principal variables:

Symbol	*Type*	*Description*
ADDY	real	Sum of stage vapor-phase mole fractions
TJ	real	Stage temperature, T

Subroutine SETUPB

This subroutine computes the coefficients, AA, of the tridiagonal stage heat-balance matrix for the application of the Newton-Raphson method. Thus, including the constant vector, the matrix has the dimensions, JS by (JS + 1). A description of the matrix equations is given on page 170 of the Burningham-Otto article. These equations involve stream enthalpies and derivatives of enthalpies with respect to temperature, which are computed, respectively, by function subprograms HVL and HDRV, as described below.

Subprograms called:

Name	*Type*	*Purpose*
HVL	real function	Computes molal enthalpies for vapor and liquid streams
HDRV	real function	Computes derivatives of vapor and liquid enthalpies with respect to temperature; these derivatives are obtained from Equations 3 and 5 above.

Subroutine DELTAT

This subroutine solves the Newton-Raphson form of the heat-balance matrix equations for the stage-temperature changes, ΔT_j. The new stage temperatures are then computed from

$$\left(T_j\right)_{new} = \left(T_j\right)_{old} + \left(\Delta T_j\right).$$

The iterative procedure is continued until successive temperature differences deviate by less than 0.1°F or until a maximum of NHBI iterations is reached. A modified Gauss elimination procedure is used in a manner analogous to that used in TRIDI.

Principal variable:

Symbol	*Type*	*Description*
DELT	real	Stage-temperature change from one column iteration to the next

Miscellaneous Comments Concerning Subprograms

A separate subprogram is not provided for computing component liquid and vapor enthalpies. Instead, they are calculated where required in FEEDH and HVL.

Sample Problem

The application of STAB may be illustrated by obtaining the solution to the problem stated in the section, "Technical Description." This example makes use of only a few of the features of STAB. An echo print of the data is shown after the FØRTRAN program listing given below. The K-value coefficients were obtained by fitting polynomial equations to available data at 75 psia. The absorber oil was assumed to have the properties of n-dodecane. Except for methane and the absorber oil, the enthalpy coefficients were those given by Amundson and Pontinen.[24] The other enthalpy coefficients were obtained by fitting polynomial equations to available data. All the physical properties are judged to be valid over a temperature range of 50°F to 150°F. Below 50°F, negative K values are possible for the absorber oil. A value of 2 for KP will cause intermediate results to be printed every two column iterations. A maximum of 15 column iterations is permitted, because no value of NCI is specified in the data input.

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[24] Amundson and Pontinen, *loc. cit.*

The problem statement in the section, "Technical Description," gives the gas-flow rate as 18,000,000 SCFD (60°F and 1 atm) and an absorber-oil rate of 300,000 gal/day. These were converted by hand calculations to 1978.45 lbmoles/hr of feed gas and 533.0 lbmoles/hr of feed liquid.

The results of the calculations for the sample problem are given following the echo print of the input data, except that only one summary of intermediate results is included.

FØRTRAN Program Listing: Main Program Followed by Subprograms

```
C-----MAIN PROGRAM FOR          S T A B                                 MAIN0001
C-----MULTICOMPONENT STRIPPING AND ABSORPTION                           MAIN0002
C-----WRITTEN BY T. SHINOHARA, P.J. JOHANSEN AND J.D. SEADER, U. OF UTAHMAIN0003
C-----LAST REVISION -   JUNE, 1972                                      MAIN0004
      REAL KCONST, L                                                    MAIN0005
      INTEGER PHASE                                                     MAIN0006
      EXTERNAL EQUILK                                                   MAIN0007
      DIMENSION TS(100),TTS(100),XFEED(20),JP(20),PH(2),AK(20),HV(20),  MAIN0008
     1 HL(20)                                                           MAIN0009
      COMMON/BLOCK1/JS,T(100),F(100),W(100),U(100),V(100),XF(20,100)    MAIN0010
      COMMON/AA1/TF(100),HF(100),Q(100)                                 MAIN0011
      COMMON/AA2/HVCNST(3,20),HLCNST(3,20),IC,L(100)                    MAIN0012
      COMMON/AA3/TD,TB,KCONST(4,20)                                     MAIN0013
      COMMON/AA4/X(20,100)                                              MAIN0014
      COMMON/AA5/Z(20,100),ZY(20,100),ADDX(100),Y(20,100)               MAIN0015
C-----ASSIGN INPUT/OUTPUT DEVICE NUMBERS,ITERATION LIMIT,  AND TOLERANCEMAIN0016
      DATA LUIN, LUOUT, NHBI, TAL/5,6,15,.01/                           MAIN0017
      DATA PH(1), PH(2)/3HVAP,3HLIQ/                                    MAIN0018
      READ (LUIN,220) IC, TLOW, THI, P, NCI                             MAIN0019
      IF (NCI .EQ. 0) NCI = 15                                          MAIN0020
      WRITE (LUOUT,215) NHBI,NCI,TAL                                    MAIN0021
      TT = (THI + TLOW)/2.                                              MAIN0022
      WRITE (LUOUT,235) P,TLOW, THI, TT                                 MAIN0023
      IF (IC .GT. 1 .AND. IC .LE. 20) GO TO 5                           MAIN0024
      WRITE (LUOUT,410)                                                 MAIN0025
      GO TO 190                                                         MAIN0026
C-----READ IN AND PRINT THE PHYSICAL PROPERTY DATA                      MAIN0027
    5 READ (LUIN,225) ((KCONST(IK,JK), IK = 1,4), JK =1, IC)            MAIN0028
      READ (LUIN, 230) ((HVCNST(IK, JK), IK = 1,3), JK = 1,IC)          MAIN0029
      READ (LUIN, 230) ((HLCNST(IK, JK), IK = 1,3), JK = 1, IC)         MAIN0030
      DO 10 JK = 1,IC                                                   MAIN0031
      AK(JK) = EQUILK(TT,JK)                                            MAIN0032
      HV(JK) = HVCNST(1,JK) + HVCNST(2,JK)*TT + HVCNST(3,JK)*TT*TT      MAIN0033
      HL(JK) = HLCNST(1,JK) + HLCNST(2,JK)*TT + HLCNST(3,JK)*TT*TT      MAIN0034
   10 CONTINUE                                                          MAIN0035
      WRITE (LUOUT,240) (JK,(KCONST(IK,JK),IK=1,4), AK(JK), JK=1,IC)    MAIN0036
      WRITE (LUOUT,245) (JK,(HVCNST(IK,JK),IK=1,3), HV(JK), JK=1,IC)    MAIN0037
      WRITE (LUOUT,250) (JK,(HLCNST(IK,JK),IK=1,3), HL(JK), JK=1,IC)    MAIN0038
C-----READ IN AND PRINT DATA FOR A CASE                                  MAIN0039
   15 READ (LUIN, 255) NC, JS, NOF, NOVS, NOLS, NOQS, KP                MAIN0040
      IF (KP .EQ. 0) KP = 10                                            MAIN0041
      IF (JS .GT. 2 .AND. JS .LE. 100) GO TO 20                         MAIN0042
      WRITE (LUOUT,420)                                                 MAIN0043
      GO TO 190                                                         MAIN0044
C-----ZERO OUT CERTAIN ARRAYS BEFORE STARTING A CASE                      MAIN0045
   20 CALL CLEAN                                                        MAIN0046
      TOL = TAL * JS                                                    MAIN0047
      READ (LUIN,260) TB,TD                                             MAIN0048
      WRITE (LUOUT,265) NC,IC,JS,NOF,NOVS,NOLS,NOQS,TD,TB               MAIN0049
      WRITE (LUOUT,270) IC                                              MAIN0050
      SUMFD = 0.0                                                       MAIN0051
      DO 35 L1 = 1, NOF                                                 MAIN0052
      READ (LUIN, 275) JF, PHASE, TEMP, XFLOW                           MAIN0053
      READ (LUIN, 280) (XFEED(L2), L2 = 1, IC)                          MAIN0054
      WPHASE = PH(1)                                                    MAIN0055
      IF (PHASE .EQ. 2) WPHASE = PH(2)                                  MAIN0056
      WRITE (LUOUT,285) JF, XFLOW, WPHASE, TEMP, (XFEED(L2), L2=1,IC)   MAIN0057
      SUMMF = 0.0                                                       MAIN0058
      DO 25 M = 1, IC                                                   MAIN0059
      SUMMF = SUMMF + XFEED(M)                                          MAIN0060
   25 CONTINUE                                                          MAIN0061
      IF (SUMMF .LT. 0.999 .OR. SUMMF .GT. 1.001) WRITE (LUOUT,425) JF  MAIN0062
      IF (SUMMF .LT. 0.999 .OR. SUMMF .GT. 1.001) WRITE (LUOUT,430)     MAIN0063
      TF(JF) = TEMP                                                     MAIN0064
      F(JF) = XFLOW                                                     MAIN0065
      JP(JF) = PHASE                                                    MAIN0066
      SUMFD = SUMFD + F(JF)                                             MAIN0067
      DO 30 L2 = 1, IC                                                  MAIN0068
      XF(L2,JF) = XFEED(L2)                                             MAIN0069
   30 CONTINUE                                                          MAIN0070
C-----COMPUTE FEED ENTHALPY                                               MAIN0071
      HF(JF) = FEEDH (PHASE, JF)                                        MAIN0072
   35 CONTINUE                                                          MAIN0073
      KKK = 0                                                           MAIN0074
      IF (NOVS .EQ. 0) GO TO 45                                         MAIN0075
      WPHASE = PH(1)                                                    MAIN0076
      WRITE (LUOUT, 290)                                                MAIN0077
      KKK = 1                                                           MAIN0078
      DO 40 L3 = 1, NOVS                                                MAIN0079
      READ (LUIN, 220) JSV, VRATE                                       MAIN0080
      WRITE (LUOUT, 295) JSV, VRATE, WPHASE                             MAIN0081
      IF (JSV .LT. 2 .OR. JSV .GT. (JS-1)) GO TO 190                    MAIN0082
      W(JSV) = VRATE                                                    MAIN0083
   40 CONTINUE                                                          MAIN0084
   45 IF (NOLS .EQ. 0) GO TO 55                                         MAIN0085
      WPHASE = PH(2)                                                    MAIN0086
      IF (KKK .EQ. 0) WRITE (LUOUT,290)                                 MAIN0087
      DO 50 L4 = 1, NOLS                                                MAIN0088
      READ (LUIN, 220) JSL, RATE                                        MAIN0089
      WRITE (LUOUT, 295) JSL, RATE, WPHASE                              MAIN0090
      IF (JSL .LT. 2 .OR. JSL .GT. (JS-1)) GO TO 190
      U(JSL) = RATE
   50 CONTINUE
   55 IF (NOQS .EQ. 0) GO TO 65
      WRITE (LUOUT, 300)
      DO 60 L5 = 1, NOQS
      READ (LUIN, 305) JQ, QRATE
      WRITE (LUOUT, 310) JQ, QRATE
      IF (JQ .LT. 2 .OR. JQ .GT. (JS-1)) GO TO 190
      Q(JQ) = QRATE
   60 CONTINUE
C-----COMPUTE INITIAL TEMPERATURE AND VAPOR RATE PROFILES
   65 CALL ASUMVT(JP)
      WRITE (LUOUT,315)
      WRITE (LUOUT,320) (I, T(I), V(I), I= 1,JS)
      WRITE (LUOUT,325) KP
C-----COMPUTE INITIAL LIQUID RATE PROFILE
      JL1 = JS - 1
       SUM = 0.0
      DO 70 I=1,JL1
      SUM = SUM + F(I) - W(I) - U(I)
      L(I) = V(I+1)+SUM-V(1)
      TS(I) = T(I)
      TTS(I) = T(I)
   70 CONTINUE
      L(JS) = SUM + F(JS) -W(JS) -U(JS) - V(1)
      TS(JS) = T(JS)
      TTS(JS) = T(JS)
      K2 = 0
      K1= 0
   75 K1 = K1 + 1
      K2 = K2 + 1
C-----COMPUTE MATRIX COEFFICIENTS FOR LIQUID MOLE FRACTIONS
      DO 80 I = 1, IC
      CALL SETUPA (I,EQUILK)
C-----SOLVE MATRIX FOR LIQUID MOLE FRACTIONS
      CALL TRIDI(I)
   80 CONTINUE
C-----COMPUTE VAPOR MOLE FRACTIONS, AND VAPOR AND LIQUID RATE PROFILES
      CALL VAPOR(EQUILK)
      DO 100 I=1,NHBI
C-----COMPUTE MATRIX COEFFICIENTS FOR TEMPERATURE CHANGES
      CALL SETUPB
C-----COMPUTE NEW STAGE TEMPERATURES
      CALL DELTAT
      IF(I.EQ.1) GO TO 90
      DO 85 J=1,JS
      IF(ABS(T(J)-TTS(J)) .GT. .1) GO TO 90
   85 CONTINUE
      GO TO 105
   90 DO 95 J=1,JS
      TTS(J)=T(J)
   95 CONTINUE
  100 CONTINUE
  105 IF (T(J) .LT. TLOW .OR. T(J) .GT. THI) GO TO 195
      DO 110 J=1,JS
      IF(V(J).LT.0.0) GO TO 200
      IF(L(J).LT.0.0) GO TO 210                                         MAIN0148
  110 CONTINUE                                                          MAIN0149
      IF (K2 .NE. KP .AND. K1 .NE. NCI) GO TO 130                       MAIN0150
      WRITE (LUOUT,350)                                                 MAIN0151
      WRITE (LUOUT,330) K1, IC                                          MAIN0152
      K2 = 0                                                            MAIN0153
C-----COMPUTE SUM OF LIQUID MOLE FRACTIONS                               MAIN0154
      DO 125 I=1,JS                                                     MAIN0155
  115 ADD = 0.0                                                         MAIN0156
      DO 120 K = 1, IC                                                  MAIN0157
      ADD = ADD + X(K,I)                                                MAIN0158
  120 CONTINUE                                                          MAIN0159
      WRITE (LUOUT, 335) I, T(I), V(I), L(I), (X(K, I), K = 1, IC)      MAIN0160
      WRITE (LUOUT, 340) ADD                                            MAIN0161
      WRITE (LUOUT, 345) (Y(K, I), K = 1, IC)                           MAIN0162
  125 CONTINUE                                                          MAIN0163
C-----CONVERGENCE TEST                                                   MAIN0164
  130 STD = 0.0                                                         MAIN0165
      DO 135 J = 1, JS                                                  MAIN0166
      DIFF = T(J) - TS(J)                                               MAIN0167
      TS(J) = T(J)                                                      MAIN0168
      STD = STD + DIFF * DIFF                                           MAIN0169
  135 CONTINUE                                                          MAIN0170
      IF(STD.GT.TOL .AND. K1.LT.NCI) WRITE(LUOUT,355) K1,STD,TOL        MAIN0171
      IF (STD .GT. TOL .AND. K1 .LT. NCI) GO TO 75                      MAIN0172
      IF (STD.LE.TOL)  GO TO 140                                        MAIN0173
      IF (K1 .EQ. NCI) WRITE (LUOUT,365) NCI                            MAIN0174
      GO TO 145                                                         MAIN0175
  140 WRITE (LUOUT, 360) K1, STD, TOL                                   MAIN0176
  145 WRITE (LUOUT,370) IC                                              MAIN0177
      WRITE (LUOUT,375) PH(1),T(1),V(1),(Y(K,1),K=1,IC)                 MAIN0178
      JSS = JS - 1                                                      MAIN0179
      IF (NOVS .EQ. 0) GO TO 155                                        MAIN0180
      DO 150 I=2,JSS                                                    MAIN0181
      IF (W(I) .LT. .00001) GO TO 150                                   MAIN0182
      WRITE (LUOUT,380) I, PH(1), T(1), W(I), (Y(K,I), K=1,IC)          MAIN0183
  150 CONTINUE                                                          MAIN0184
  155 IF (NOLS .EQ. 0) GO TO 165                                        MAIN0185
      DO 160 I=2,JSS                                                    MAIN0186
      IF (U(I) .LT. .00001) GO TO 160                                   MAIN0187
      WRITE (LUOUT,380) I, PH(2), T(I), U(I), (X(K,I), K=1,IC)          MAIN0188
  160 CONTINUE                                                          MAIN0189
  165 WRITE (LUOUT,385) JS, PH(2), T(JS),L(JS),(X(K,JS),K=1,IC)         MAIN0190
  170 WRITE (LUOUT,350)                                                 MAIN0191
  175 WRITE (LUOUT,395) IC,IC                                           MAIN0192
      DO 185 I=1,JS                                                     MAIN0193
      IF (I.EQ.1) GO TO 180                                             MAIN0194
      WRITE (LUOUT,400) I, T(I), V(I), (Y(K,I), K=1,IC)                 MAIN0195
      IF (I.EQ.JS) GO TO 185                                            MAIN0196
  180 WRITE (LUOUT,405) I, T(I), L(I), (X(K,I), K=1,IC)                 MAIN0197
  185 CONTINUE                                                          MAIN0198
      GO TO 15                                                          MAIN0199
  190 WRITE (LUOUT,415)                                                 MAIN0200
      STOP                                                              MAIN0201
  195 WRITE (LUOUT,435) T(J), J, K1                                     MAIN0202
      WRITE (LUOUT,440)                                                 MAIN0203
      STOP                                                              MAIN0204
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200 WRITE (LUOUT,445) V(J),J,K1                                         MAIN0205
    WRITE (LUOUT,450)                                                   MAIN0206
205 WRITE (LUOUT,460)                                                   MAIN0207
    GO TO 15                                                            MAIN0208
210 WRITE (LUOUT,455) L(J), J, K1                                       MAIN0209
    WRITE (LUOUT,450)                                                   MAIN0210
    GO TO 205                                                           MAIN0211
215 FORMAT (1H1///////56X,9H S T A B /////////40X,39HMULTICOMPONENT STMAIN0212
   1RIPPING AND ABSORPTION/////////,30X,60HMAXIMUM NUMBER OF ITERATIONSMAIN0213
   2 FOR TEMPERATURE CALCULATIONS = ,I3////30X,38HMAXIMUM NUMBER OF COMAIN0214
   3LUMN ITERATIONS = ,I4////30X,54HCONSTANT FOR COLUMN ITERATION CONVMAIN0215
   4ERGENCE CRITERION = ,F7.5/1H1)                                      MAIN0216
220 FORMAT (I10,3F10.2, I10)                                            MAIN0217
225 FORMAT (4E15.5)                                                     MAIN0218
230 FORMAT (3E15.5)                                                     MAIN0219
235 FORMAT (//33X,54HCOEFFICIENTS OF POLYNOMIAL PHYSICAL-PROPERTY EQUAMAIN0220
   1TIONS//41X,38HPROPERTY = A + B*T + C*T**2. + D*T**3./48X,16HWITH TMAIN0221
   2 IN DEG. F///41X,11HPRESSURE = ,F8.3,6H  PSIA//41X,26HVALID TEMPERMAIN0222
   3ATURE RANGE = ,F8.2,4H TO ,F8.2,8H  DEG. F////101X,14HPROPERTY VALMAIN0223
   4UE/25X,9HCOMPONENT,8X,1HA,14X,1HB,14X,1HC,14X,1HD,11X,3HAT ,F8.2,7MAIN0224
   5H DEG. F/25X,9H---------,3X,11H-----------,4X,11H-----------,4X,11MAIN0225
   6H-----------,4X,11H-----------, 6X,18H------------------//)         MAIN0226
240 FORMAT (10X,9HK-VALUES /(26X,I5,2X,4E15.5,6X,F15.5)/)               MAIN0227
245 FORMAT (10X,16HVAPOR ENTHALPIES/10X,13H(BTU/LBMOLE) /(26X,I5,2X,3EMAIN0228
   115.5,21X,F15.5)/)                                                   MAIN0229
250 FORMAT (10X,17HLIQUID ENTHALPIES/10X,13H(BTU/LBMOLE) /(26X,I5,2X,3MAIN0230
   1E15.5,21X,F15.5)/)                                                  MAIN0231
255 FORMAT (8I10)                                                       MAIN0232
260 FORMAT (2F10.2)                                                     MAIN0233
265 FORMAT (1H1//53X,11HCASE NUMBER,I10////35X,29HNO. OF CHEMICAL COMPMAIN0234
   1ONENTS = ,I5//35X,28HNO. OF THEORETICAL STAGES = ,I5//35X,15HNO. OMAIN0235
   2F FEEDS = ,I5//35X,27HNO. OF VAPOR SIDESTREAMS = ,I5//35X,28HNO. OMAIN0236
   3F LIQUID SIDESTREAMS = ,I5//35X,30HNO. OF HEAT-TRANSFER STAGES = ,MAIN0237
   4I5//35X,46HESTIMATED TOP AND BOTTOM STAGE TEMPERATURES ARE ,F10.2,MAIN0238
   54H AND,F10.2,7H DEG. F////35X,38HSTAGES ARE NUMBERED DOWN FROM THEMAIN0239
   6 TOP./1H1)                                                          MAIN0240
270 FORMAT (///32X,55HFEED, SIDESTREAM, AND HEAT-TRANSFER RATE SPECIFIMAIN0241
   1CATIONS///56X,13HHEAT-TRANSFER/23X, 9HFLOW RATE,6X,5HPHASE,5X,5HTEMAIN0242
   2MP.,8X,4HRATE/15X,5HSTAGE,2X,12H(LBMOLES/HR),2X, 9HCONDITION,2X,8HMAIN0243
   3(DEG. F),3X,8H(BTU/HR),7X,44HCOMPONENT MOLE FRACTIONS FOR COMPONENMAIN0244
   4TS 1 TO,I3/                                                         MAIN0245
   5                                                     15X,105H----MAIN0246
   6- ------------ -------- -------- -------------  -------------MAIN0247
   7-------------------------------------------------//5X,6HFEEDS /) MAIN0248
275 FORMAT (2I10,2F10.2)                                                MAIN0249
280 FORMAT (5F10.5)                                                     MAIN0250
285 FORMAT (14X,I5,F15.5,4X,A4,2X,F10.2,16X,5F10.5/(70X,5F10.5 )//)     MAIN0251
290 FORMAT (5X,12HSIDESTREAMS /)                                        MAIN0252
295 FORMAT (14X,I5,F15.5,4X,A4/)                                        MAIN0253
300 FORMAT (5X,14HHEAT TRANSFER,/3X,16H(-) IF TO STAGE,/3X,18H(+) IF FMAIN0254
   1ROM STAGE /)                                                        MAIN0255
305 FORMAT (I10,F15.5)                                                  MAIN0256
310 FORMAT (15X,I5,33X,E15.5/)                                          MAIN0257
315 FORMAT (1H1///40X,39HSTAGE TEMPERATURES AND VAPOR FLOW RATES//43X,MAIN0258
   136HUSED TO INITIALIZE COLUMN ITERATIONS///49X,11HTEMPERATURE,10X,1MAIN0259
   20HVAPOR RATE/38X,5HSTAGE,8X,8H(DEG. F),10X,12H(LBMOLES/HR)/38X,5H-MAIN0260
   3----,6X,12H------------,8X,12H------------/)                        MAIN0261
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320 FORMAT (   38X,I5,7X,F10.2,6X,F15.5)                              MAIN0262
325 FORMAT (/9X,46HINTERMEDIATE RESULTS WILL BE PRINTED OUT EVERY,I5,2MAIN0263
    1X,17HCOLUMN ITERATIONS/)                                         MAIN0264
330 FORMAT (40X,34HINTERMEDIATE RESULTS FOR ITERATION,I4///13X,5HTEMP.MAIN0265
    1,5X,10HVAPOR RATE,4X,11HLIQUID RATE,4X,40HLIQUID, FOLLOWED BY VAPOMAIN0266
    2R,MOLE FRACTIONS,10X,11HLIQUID MOLE/5X,5HSTAGE,2X,8H(DEG. F),2X,12MAIN0267
    3H(LBMOLES/HR),3X,12H(LBMOLES/HR),5X,15HCOMPONENTS 1 TO,I3,30X,12HFMAIN0268
    4RACTION SUM/5X,5H-----,2X,8H--------,2X,12H------------,3X,12H----MAIN0269
    5--------,3X,47H-----------------------------------------------,3X,MAIN0270
    612H------------)                                                 MAIN0271
335 FORMAT (4X,I4,2X,F9.2,F15.5,F15.5,5F10.5/(49X,5F10.5))            MAIN0272
340 FORMAT ( 99X,F10.5)                                               MAIN0273
345 FORMAT  (49X,5F10.5)                                              MAIN0274
350 FORMAT (1H1)                                                      MAIN0275
355 FORMAT (/20X,15HAFTER ITERATION,I5,2X,31HCALCULATIONS ARE NOT CONVMAIN0276
    1ERGED./20X,38HCOLUMN ITERATION CONVERGENCE FACTOR IS,E15.5,2X,36H,MAIN0277
    2 WHICH IS GREATER THAN TOLERANCE OF,F10.5)                       MAIN0278
360 FORMAT (/20X,15HAFTER ITERATION,I5,2X,27HCALCULATIONS ARE CONVERGEMAIN0279
    1D./20X,26HCOLUMN ITERATION FACTOR IS,F10.5,2X,33H  WHICH IS LESS TMAIN0280
    2HAN TOLERANCE OF,F10.5/20X,43HFINAL DETAILED RESULTS WILL NOW BE PMAIN0281
    3RINTED.)                                                         MAIN0282
365 FORMAT (/20X,91HCALCULATIONS ARE NOT CONVERGED AFTER MAXIMUM NUMBEMAIN0283
    1R OF COLUMN ITERATIONS, NCI, SPECIFIED AS,I5/20X,78HDETAILED UNCONMAIN0284
    2VERGED RESULTS WILL NOW BE PRINTED SO USER CAN DETERMINE WHETHER/2MAIN0285
    30X,59HIT IS WORTHWHILE TO REPEAT CASE WITH A LARGER VALUE OF NCI.)MAIN0286
370 FORMAT (1H1////53X,13HFINAL RESULTS//42X,36HPRODUCT STREAMS AND EXMAIN0287
    1CHANGER DUTIES//16X,4HFROM,3X,5HPHASE,5X,5HTEMP.,5X,9HFLOW RATE,8XMAIN0288
    2,24HCOMPONENT MOLE FRACTIONS/7X,6HSTREAM,2X,5HSTAGE,1X,9HCONDITIONMAIN0289
    3,1X,8H(DEG. F),3X,12H(LBMOLES/HR),6X,19HFOR COMPONENTS 1 TO,I4/7X,MAIN0290
    46H------,2X,5H-----,1X,8H--------,2X,8H--------,3X,11H-----------,MAIN0291
    53X,48H------------------------------------------------/)         MAIN0292
375 FORMAT (5X,7HGAS OUT,5X,2H 1,5X,A4,1X,F10.2,F15.5,5F10.5/(54X,5F10MAIN0293
    1.5)/)                                                            MAIN0294
380 FORMAT (4X,10HSIDESTREAM,2X,I3,5X,A4,1X,F10.2,F15.5,5F10.5/(55X,5FMAIN0295
    110.5)/)                                                          MAIN0296
385 FORMAT (5X,7HLIQ OUT,4X,I3,5X,A4,1X,F10.2,F15.5,5F10.5/(54X,5F10.5MAIN0297
    1)/)                                                              MAIN0298
390 FORMAT (20X,17HCONDENSER DUTY = ,E15.5, 8H  BTU/HR/20X,18HREBOILERMAIN0299
    1 DUTY =   ,E15.5, 8H  BTU/HR/1H1)                                MAIN0300
395 FORMAT (////53X,13HFINAL RESULTS//51X,19HINTERNAL CONDITIONS//27X,MAIN0301
    117HFLOWS FROM STAGES/13X,5HTEMP.,5X,10HVAPOR RATE,4X,11HLIQUID RATMAIN0302
    2E,4X,21HLIQUID MOLE FRACTIONS,19X,20HVAPOR MOLE FRACTIONS/5X,5HSTAMAIN0303
    3GE,2X,8H(DEG. F),2X,12H(LBMOLES/HR),3X,12H(LBMOLES/HR),3X,16HCOMPOMAIN0304
    4NENTS 1 TO ,I4,20X,16HCOMPONENTS 1 TO ,I4/5X,5H-----,2X,9H--------MAIN0305
    5-,2X,12H------------,3X,12H------------,2X,38H-------------------MAIN0306
    6-------------------,2X,38H--------------------------------------//)MAIN0307
400 FORMAT (5X,I4,1X,F10.2,F15.5,55X,5F8.5/(90X,5F8.5))               MAIN0308
405 FORMAT (5X,I4,1X,F10.2,15X,F15.5,5F8.5/(50X,5F8.5))               MAIN0309
410 FORMAT (20X,70HNUMBER OF CHEMICAL SPECIES ARE NOT WITHIN LIMITS OFMAIN0310
    1 PROGRAM DIMENSION.)                                             MAIN0311
415 FORMAT (20X,32HDATA INPUT MAY CONTAIN ERROR(S).,39HCAREFULLY CHECKMAIN0312
    1 PRINTOUT OF INPUT DATA./20X,38HDATA CARDS MAY NOT BE IN PROPER ORMAIN0313
    2DER./5X,19HPROGRAM TERMINATED.)                                  MAIN0314
420 FORMAT (20X,60HNUMBER OF STAGES ARE NOT WITHIN LIMITS OF PROGRAM DMAIN0315
    1IMENSION.)                                                       MAIN0316
425 FORMAT (20X,29HFEED MOLE FRACTIONS FOR STAGE,I4,20H DO NOT SUM TO MAIN0317
    11.000)                                                           MAIN0318
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430 FORMAT (20X,87HCALCULATIONS ALLOWED TO PROCEED, BUT THEY MAY NOT CMAIN0319
   1ONVERGE OR THEY MAY NOT BE ACCURATE.)                             MAIN0320
435 FORMAT (20X,24HCOMPUTED TEMPERATURE OF ,F10.2,2X,17HDEG. F, FOR STMAIN0321
   1AGE,I4/20X,19HOF COLUMN ITERATION,I4,68H, IS OUTSIDE OF RANGE OF VMAIN0322
   2ALIDITY OF PHYSICAL PROPERTY COEFFICIENTS.)                       MAIN0323
440 FORMAT (20X,59HSHOULD REPEAT RUN WITH VALID PHYSICAL PROPERTY COEFMAIN0324
   1FICIENTS/5X,19HPROGRAM TERMINATED.)                               MAIN0325
445 FORMAT (20X,22HCOMPUTED VAPOR RATE OF,F15.5,10H FOR STAGE,I4,2X,19MAIN0326
   1HOF COLUMN ITERATION,I4,2X,12HIS NEGATIVE.)                       MAIN0327
450 FORMAT (20X,78HTHIS MAY BE DUE TO IMPROPER FEED, SIDESTREAM, OR HEMAIN0328
   1AT TRANSFER SPECIFICATIONS,/20X,45HCAUSING IMPOSSIBLE MATERIAL OR MAIN0329
   2HEAT BALANCES. /5X,16HCASE TERMINATED.)                           MAIN0330
455 FORMAT (20X,23HCOMPUTED LIQUID RATE OF,F15.5,10H FOR STAGE,I4,2X,1MAIN0331
   19HOF COLUMN ITERATION,I4,2X,12HIS NEGATIVE.)                      MAIN0332
460 FORMAT (20X,46HSHOULD REPEAT RUN WITH REVISED SPECIFICATIONS./)   MAIN0333
    END                                                               MAIN0334
```

```
    SUBROUTINE ASUMVT(JP)                                             ASUM0001
    DIMENSION JP(20)                                                  ASUM0002
    COMMON/BLOCK1/JS,T(100),F(100),W(100),U(100),V(100),XF(20,100)    ASUM0003
    COMMON /AA3/TD,TB,KCONST(4,20)                                    ASUM0004
    JK=JS-1                                                           ASUM0005
    V(JS)=F(JS)-W(JS)                                                 ASUM0006
    DO 10 I=1,JK                                                      ASUM0007
    K=JS-I                                                            ASUM0008
    IF (JP(K).EQ.2) GO TO 5                                           ASUM0009
    V(K)=V(K+1)+F(K)-W(K)                                             ASUM0010
    GO TO 10                                                          ASUM0011
  5 V(K)=V(K+1)-W(K)                                                  ASUM0012
 10 CONTINUE                                                          ASUM0013
    TINK=(TB-TD)/JK                                                   ASUM0014
    T(1)=TD                                                           ASUM0015
    DO 15 L1=2,JS                                                     ASUM0016
    T(L1)=T(L1-1)+TINK                                                ASUM0017
 15 CONTINUE                                                          ASUM0018
    RETURN                                                            ASUM0019
    END                                                               ASUM0020
```

```
      SUBROUTINE CLEAN
      COMMON/BLOCK1/JS,T(100),F(100),W(100),U(100),V(100),XF(20,100)
      COMMON /AA1/TF(100),HF(100),Q(100)
      DO 5 I=1,100
      F(I)=0.0
      TF(I)=0.0
      HF(I)=0.0
      W(I)=0.0
      U(I)=0.0
      Q(I)=0.0
    5 CONTINUE
      DO 15 J=1,100
      DO 10 I=1,20
      XF(I,J)=0.0
   10 CONTINUE
   15 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE DELTAT
      DIMENSION P(100),QA(100)
      DIMENSION DELT(100)
      COMMON/BLOCK1/JS,T(100),F(100),W(100),U(100),V(100),XF(20,100)
      COMMON /AA2/AA(100,101)
      M1=JS+1
      P(1)=AA(1,2)/AA(1,1)
      QA(1)=AA(1,M1)/AA(1,1)
      NMIN=JS-1
      DO 5 J1=2,JS
      P(J1)=AA(J1,J1+1)/(AA(J1,J1)-AA(J1,J1-1)*P(J1-1))
      QA(J1)=(AA(J1,M1)-AA(J1,J1-1)*QA(J1-1))/(AA(J1,J1)-AA(J1,J1-1)
     1*P(J1-1))
    5 CONTINUE
      DELT(JS)=QA(JS)
      DO 10 J1=1,NMIN
      JSUB=NMIN-J1+1
      DELT(JSUB)=QA(JSUB)-P(JSUB)*DELT(JSUB+1)
   10 CONTINUE
      DO 15 J2=1,JS
      T(J2)=DELT(J2)+T(J2)
   15 CONTINUE
      RETURN
      END
```

```
      FUNCTION EQUILK(TT,I)
      REAL KCONST
      COMMON /AA3/TD,TB,KCONST(4,20)
      EQUILK=KCONST(1,I)+KCONST(2,I)*TT+KCONST(3,I)*TT*TT
     1+KCONST(4,I)*TT*TT*TT
      RETURN
      END
      FUNCTION FEEDH(KPHASE,JF)                                         FEED0001
      COMMON/BLOCK1/JS,T(100),F(100),W(100),U(100),V(100),XF(20,100)    FEED0002
      COMMON /AA1/TF(100),HF(100),Q(100)                                FEED0003
      COMMON /AA2/HVCNST(3,20),HLCNST(3,20),IC,L(100)                   FEED0004
      IF (KPHASE.EQ.1) GO TO 10                                         FEED0005
      FEEDH=0.0                                                         FEED0006
      DO 5 I1=1,IC                                                      FEED0007
      FEEDH=FEEDH+XF(I1,JF)*(HLCNST(1,I1)+HLCNST(2,I1)*TF(JF)           FEED0008
     1+HLCNST(3,I1)*TF(JF)*TF(JF))                                      FEED0009
    5 CONTINUE                                                          FEED0010
      RETURN                                                            FEED0011
   10 FEEDH=0.0                                                         FEED0012
      DO 15 I1=1,IC                                                     FEED0013
      FEEDH=FEEDH+XF(I1,JF)*(HVCNST(1,I1)+HVCNST(2,I1)*TF(JF)           FEED0014
     1+HVCNST(3,I1)*TF(JF)*TF(JF))                                      FEED0015
   15 CONTINUE                                                          FEED0016
      RETURN                                                            FEED0017
      END                                                               FEED0018
```

```
      FUNCTION HDRV(K,TT,JJ)                                            HDRV0001
      COMMON /AA2/HVCNST(3,20),HLCNST(3,20),IC,L(100)                   HDRV0002
      COMMON /AA5/Z(20,100),ZY(20,100),ADDX(100),Y(20,100)              HDRV0003
      HDRV=0.0                                                          HDRV0004
      IF (K.EQ.1) GO TO 10                                              HDRV0005
      DO 5 I=1,IC                                                       HDRV0006
      HDRV=HDRV+ZY(I,JJ)*(HVCNST(2,I)+2.*HVCNST(3,I)*TT)                HDRV0007
    5 CONTINUE                                                          HDRV0008
      RETURN                                                            HDRV0009
   10 CONTINUE                                                          HDRV0010
      DO 15 I=1,IC                                                      HDRV0011
      HDRV=HDRV+Z(I,JJ)*(HLCNST(2,I)+2.*HLCNST(3,I)*TT)                 HDRV0012
   15 CONTINUE                                                          HDRV0013
      RETURN                                                            HDRV0014
      END                                                               HDRV0015
```

```
      FUNCTION HVL(K,TT,JJ)                                             HVL 0001
      COMMON /AA2/HVCNST(3,20),HLCNST(3,20),IC,L(100)                   HVL 0002
      COMMON /AA5/Z(20,100),ZY(20,100),ADDX(100),Y(20,100)              HVL 0003
      HVL = 0.0                                                         HVL 0004
      IF (K.EQ.1) GO TO 10                                              HVL 0005
      DO 5 I=1,IC                                                       HVL 0006
      HVL=HVL+ZY(I,JJ)*(HVCNST(1,I)+HVCNST(2,I)*TT+HVCNST(3,I)*TT*TT)   HVL 0007
    5 CONTINUE                                                          HVL 0008
      RETURN                                                            HVL 0009
   10 CONTINUE                                                          HVL 0010
      DO 15 I=1,IC                                                      HVL 0011
      HVL=HVL+Z(I,JJ)*(HLCNST(1,I)+HLCNST(2,I)*TT+HLCNST(3,I)*TT*TT)    HVL 0012
   15 CONTINUE                                                          HVL 0013
      RETURN                                                            HVL 0014
      END                                                               HVL 0015
      SUBROUTINE SETUPA (I, EQUILK)                                     SETA0001
      REAL L                                                            SETA0002
      COMMON/BLOCK1/JS,T(100),F(100),W(100),U(100),V(100),XF(20,100)    SETA0003
      COMMON /AA2/HVCNST(3,20),HLCNST(3,20),IC,L(100)                   SETA0004
      COMMON /DA1/A(100,101)                                            SETA0005
      M1=JS+1                                                           SETA0006
      DO 10 I1=1,100                                                    SETA0007
      DO 5 J=1,101                                                      SETA0008
      A(I1,J)=0.0                                                       SETA0009
    5 CONTINUE                                                          SETA0010
   10 CONTINUE                                                          SETA0011
C.....FIRST ROW ELEMENTS                                                 SETA0012
      T1=T(1)                                                           SETA0013
      A(1,1)=-V(2)-F(1)+V(1)+W(1)-(V(1)+W(1))*EQUILK(T1,I)              SETA0014
      T2=T(2)                                                           SETA0015
      A(1,2)=V(2)*EQUILK(T2,I)                                          SETA0016
      A(1,M1)=-F(1)*XF(I,1)                                             SETA0017
C.....LAST ROW ELEMENTS                                                  SETA0018
      A(JS,JS-1)=W(JS)+V(JS)+L(JS)+U(JS)-F(JS)                          SETA0019
      TT=T(JS)                                                          SETA0020
      A(JS,JS)=-L(JS)-U(JS)-(W(JS)+V(JS))*EQUILK(TT,I)                  SETA0021
      A(JS,M1)=-F(JS)*XF(I,JS)                                          SETA0022
C.....MIDDLE ROW ELEMENTS                                                SETA0023
      JMINS=JS-1                                                        SETA0024
      NSTEP=0                                                           SETA0025
      SUM=0.0                                                           SETA0026
      DO 15 J1=2,JMINS                                                  SETA0027
      SUM=SUM+F(J1-1)-W(J1-1)-U(J1-1)                                   SETA0028
      SUMB=SUM+F(J1)-W(J1)-U(J1)                                        SETA0029
      A(J1,NSTEP+1)=V(J1)+SUM-V(1)                                      SETA0030
      TJ1=T(J1)                                                         SETA0031
      A(J1,NSTEP+2)=-(V(J1)+W(J1))*EQUILK(TJ1,I)-U(J1)-V(J1+1)-SUMB+V(1)SETA0032
      TJ1P=T(J1+1)                                                      SETA0033
      A(J1,NSTEP+3)=V(J1+1)*EQUILK(TJ1P,I)                              SETA0034
      A(J1,M1)=-F(J1)*XF(I,J1)                                          SETA0035
      NSTEP=NSTEP+1                                                     SETA0036
   15 CONTINUE                                                          SETA0037
      RETURN                                                            SETA0038
      END                                                               SETA0039
      SUBROUTINE SETUPB                                                 SETB0001
      REAL L                                                            SETB0002
      COMMON/BLOCK1/JS,T(100),F(100),W(100),U(100),V(100),XF(20,100)    SETB0003
      COMMON /AA1/TF(100),HF(100),Q(100)                                SETB0004
      COMMON /AA2/HVCNST(3,20),HLCNST(3,20),IC,L(100)                   SETB0005
      COMMON /BA2/AA(100,101)                                           SETB0006
      COMMON /AA5/Z(20,100),ZY(20,100),ADDX(100),Y(20,100)              SETB0007
      M1=JS+1                                                           SETB0008
      DO 10 I=1,100                                                     SETB0009
      DO 5 J=1,101                                                      SETB0010
      AA(I,J)=0.0                                                       SETB0011
    5 CONTINUE                                                          SETB0012
   10 CONTINUE                                                          SETB0013
C.....FIRST ROW ELEMENTS EXCEPT LAST COLUMN                              SETB0014
      T1=T(1)                                                           SETB0015
      L1=1                                                              SETB0016
      L2=2                                                              SETB0017
      AA(1,1)=-(L(1)+U(1))*HDRV(L1,T1,L1)-(W(1)+V(1))*HDRV(L2,T1,L1)    SETB0018
      T2=T(2)                                                           SETB0019
      AA(1,2)=V(2)*HDRV(L2,T2,L2)                                       SETB0020
C.....LAST ROW ELEMENTS EXCEPT LAST COLUMN                               SETB0021
      TJM1=T(JS-1)                                                      SETB0022
      JAS=JS-1                                                          SETB0023
      AA(JS,JS-1)=L(JS-1)*HDRV(L1,TJM1,JAS)                             SETB0024
      TJS=T(JS)                                                         SETB0025
      AA(JS,JS)=-(L(JS)+U(JS))*HDRV(L1,TJS,JS)-(W(JS)+V(JS))*HDRV(L2,TJSSETB0026
     1,JS)                                                              SETB0027
C.....LAST COLUMN,FIRST AND LOWEST ROW                                   SETB0028
      AA(1,M1)=-V(2)*HVL(L2,T2,L2)-F(1)*HF(1)+(L(1)+U(1))*HVL(L1,T1,L1)+SETB0029
     1(W(1)+V(1))*HVL(L2,T1,L1)+Q(1)                                    SETB0030
      AA(JS,M1)=-L(JS-1)*HVL(L1,TJM1,JAS)-F(JS)*HF(JS)+(L(JS)+U(JS))*HVLSETB0031
     1(L1,TJS,JS)+(W(JS)+V(JS))*HVL(L2,TJS,JS)+Q(JS)                    SETB0032
C.....MIDDLE ELEMENTS                                                    SETB0033
      NSTEP=0                                                           SETB0034
      DO 15 J1=2,JAS                                                    SETB0035
      TT1=T(J1-1)                                                       SETB0036
      TT2=T(J1)                                                         SETB0037
      TT3=T(J1+1)                                                       SETB0038
      JJ1=J1-1                                                          SETB0039
      JJ2=J1+1                                                          SETB0040
      AA(J1,NSTEP+1)=L(JJ1)*HDRV(L1,TT1,JJ1)                            SETB0041
      AA(J1,NSTEP+2)=-(L(J1)+U(J1))*HDRV(L1,TT2,J1)-(V(J1)+W(J1))*HDRV(LSETB0042
     12,TT2,J1)                                                         SETB0043
      AA(J1,NSTEP+3)=V(JJ2)*HDRV(L2,TT3,JJ2)                            SETB0044
      AA(J1,M1)=-L(JJ1)*HVL(L1,TT1,JJ1)-V(J1+1)*HVL(L2,T(3,JJ2)-F(J1)*HFSETB0045
     1(J1)+(L(J1)+U(J1))*HVL(L1,TT2,J1)+(V(J1)+W(J1))*HVL(L2,TT2,J1)+Q(JSETB0046
     21)                                                                SETB0047
      NSTEP=NSTEP+1                                                     SETB0048
   15 CONTINUE                                                          SETB0049
      RETURN                                                            SETB0050
      END                                                               SETB0051
      SUBROUTINE TRIDI(I)                                               TRID0001
      DIMENSION P(100),QA(100)                                          TRID0002
      COMMON/BLOCK1/JS,T(100),F(100),W(100),U(100),V(100),XF(20,100)    TRID0003
      COMMON /BA1/A(100,101)                                            TRID0004
      COMMON /AA4/X(20,100)                                             TRID0005
      M1=JS+1                                                           TRID0006
      P(1)=A(1,2)/A(1,1)                                                TRID0007
      QA(1)=A(1,M1)/A(1,1)                                              TRID0008
      NMIN=JS-1                                                         TRID0009
      DO 5 J1=2,JS                                                      TRID0010
      P(J1)=A(J1,J1+1)/(A(J1,J1)-A(J1,J1-1)*P(J1-1))                    TRID0011
      QA(J1)=(A(J1,M1)-A(J1,J1-1)*QA(J1-1))/(A(J1,J1)-A(J1,J1-1)*       TRID0012
     1P(J1-1))                                                          TRID0013
    5 CONTINUE                                                          TRID0014
      X(I,JS)=QA(JS)                                                    TRID0015
      DO 10 J1=1,NMIN                                                   TRID0016
      JSUB=NMIN-J1+1                                                    TRID0017
      X(I,JSUB)=QA(JSUB)-P(JSUB)*X(I,JSUB+1)                            TRID0018
   10 CONTINUE                                                          TRID0019
      RETURN                                                            TRID0020
      END                                                               TRID0021
```

```
      SUBROUTINE VAPOR(EQUILK)                                          VAPO0001
      REAL L                                                            VAPO0002
      COMMON/BLOCK1/JS,T(100),F(100),W(100),U(100),V(100),XF(20,100)    VAPO0003
      COMMON /AA2/HVCNST(3,20),HLCNST(3,20),IC,L(100)                   VAPO0004
      COMMON /AA4/X(20,100)                                             VAPO0005
      COMMON /AA5/Z(20,100),ZY(20,100),ADDX(100),Y(20,100)              VAPO0006
      DO 15 JA=1,JS                                                     VAPO0007
      ADDX(JA)=0.0                                                      VAPO0008
      ADDY=0.0                                                          VAPO0009
      TJ=T(JA)                                                          VAPO0010
      DO 5 I=1,IC                                                       VAPO0011
      Y(I,JA)=X(I,JA)*EQUILK(TJ,I)                                      VAPO0012
      ADDX(JA)=ADDX(JA)+X(I,JA)                                         VAPO0013
      ADDY=ADDY+Y(I,JA)                                                 VAPO0014
    5 CONTINUE                                                          VAPO0015
      L(JA)=L(JA)*ADDX(JA)                                              VAPO0016
      DO 10 JB=1,IC                                                     VAPO0017
      Z(JB,JA)=X(JB,JA)/ADDX(JA)                                        VAPO0018
      ZY(JB,JA)=Y(JB,JA)/ADDY                                           VAPO0019
   10 CONTINUE                                                          VAPO0020
   15 CONTINUE                                                          VAPO0021
      V(JS)=L(JS-1)-L(JS)+F(JS)-U(JS)-W(JS)                             VAPO0022
      JK=JS-2                                                           VAPO0023
      DO 20 I=1,JK                                                      VAPO0024
      K=JS-I                                                            VAPO0025
      V(K)=V(K+1)+L(K-1)-L(K)+F(K)-U(K)-W(K)                            VAPO0026
   20 CONTINUE                                                          VAPO0027
      V(1)=V(2)-L(1)+F(1)-W(1)-U(1)                                     VAPO0028
      RETURN                                                            VAPO0029
      END                                                               VAPO0030
```

Echo Print of Input Data for Sample Problem (card columns as indicated)

```
        10        20        30        40        50        60
         1       50.      150.    75.
      1.225E+01      2.500E-01     -6.250E-04      0.000E-00
      4.750E+00     -4.270E-04      2.080E-04     -8.550E-08
      2.350E-00     -1.310E-02      1.380E-04     -8.470E-08
     -4.340E-01      1.210E-02     -1.020E-05      5.440E-08
     -2.070E-01      4.160E-03      4.770E-07      3.080E-08
     -9.000E-05      2.000E-06      0.000E-00      0.000E-00
      4.800E+03      9.000E+00      0.000E-00
     .83100E+04     .13200E+02     .60200E-02
     .11950E+05     .12350E+02     .22100E-01
     .16550E+05     .90100E+01     .37800E-01
     .19200E+05     .29500E+02     .72000E-02
      3.740E+04      4.400E+01      0.000E-00
      3.300E+03      1.100E+01      0.000E-00
     .36200E+04     .40500E+02    -.13200E-01
     .62800E+04     .25000E+02     .46500E-01
     .68400E+04     .38500E+02     .25200E-01
     .79200E+04     .43500E+02     .30200E-01
      1.280E+04      7.300E+01      0.000E-00
         6         6         2         0         0         0         2
    150.         80.
         1         2       90.      533.
    0.00        0.00      0.00      0.00      0.00
      1.
         6         1       60.   1978.45
    0.83       0.084     0.048     0.026     0.012
    0.00
```

Sample-problem Calculations--Computer Output

```
                              S T A B



                MULTICOMPONENT STRIPPING AND ABSORPTION



       MAXIMUM NUMBER OF ITERATIONS FOR TEMPERATURE CALCULATIONS =  15

       MAXIMUM NUMBER OF COLUMN ITERATIONS =   15

       CONSTANT FOR COLUMN ITERATION CONVERGENCE CRITERION =  .01000
```

```
                    COEFFICIENTS OF POLYNOMIAL PHYSICAL-PROPERTY EQUATIONS

                              PROPERTY = A + B*T + C*T**2. + D*T**3.
                                  WITH T IN DEG. F

                              PRESSURE =   75.000  PSIA

                              VALID TEMPERATURE RANGE =    50.00 TO   150.00  DEG. F

                                                                                   PROPERTY VALUE
              COMPONENT        A              B             C             D         AT   100.00 DEG. F
              ---------   -----------    -----------   -----------   -----------   -----------------

K-VALUES
                  1        .12250+02      .25000+00    -.62500-03      .00000             31.00000
                  2        .47500+01     -.42700-03     .20800-03    -.85500-07              6.70180
                  3        .23500+01     -.13100-01     .13800-03    -.84700-07              2.33530
                  4       -.43400+00      .12100-01    -.10200-04      .54400-07               .72840
                  5       -.20700+00      .41600-02     .47700-06      .30800-07               .24457
                  6       -.90000-04      .20000-05     .00000         .00000                  .00011
VAPOR ENTHALPIES
(BTU/LBMOLE)
                  1        .48000+04      .90000+01     .00060                             5700.00000
                  2        .83100+04      .13200+02     .60200-02                          9690.19995
                  3        .11950+05      .12350+02     .22100-01                         13405.99988
                  4        .16550+05      .90100+01     .37800-01                         17828.99976
                  5        .19200+05      .29500+02     .72000-02                         22221.99976
                  6        .37400+05      .44000+02     .00000                            41800.00000
LIQUID ENTHALPIES
(BTU/LBMOLE)
                  1        .33000+04      .11000+02     .00000                             4400.00000
                  2        .36200+04      .40500+02    -.13200-01                          7538.00006
                  3        .62800+04      .25000+02     .46500-01                          9244.99988
                  4        .68400+04      .38500+02     .25200-01                         10941.99988
                  5        .79200+04      .43500+02     .30200-01                         12571.99988

                  6        .12800+05      .73000+02     .00000                            20100.00000
```

```
                         CASE NUMBER         1

          NO. OF CHEMICAL COMPONENTS =     6

          NO. OF THEORETICAL STAGES =     6

          NO. OF FEEDS =     2

          NO. OF VAPOR SIDESTREAMS =     0

          NO. OF LIQUID SIDESTREAMS =     0

          NO. OF HEAT-TRANSFER STAGES =     0

          ESTIMATED TOP AND BOTTOM STAGE TEMPERATURES ARE      80.00 AND    150.00 DEG. F


          STAGES ARE NUMBERED DOWN FROM THE TOP.




                    FEED, SIDESTREAM, AND HEAT-TRANSFER RATE SPECIFICATIONS

                                                   HEAT-TRANSFER
               FLOW RATE     PHASE     TEMP.          RATE
       STAGE  (LBMOLES/HR)  CONDITION  (DEG. F)     (BTU/HR)      COMPONENT MOLE FRACTIONS FOR COMPONENTS 1 TO  6
       -----  ------------  ---------  --------  -------------   ------------------------------------------------

FEEDS

         1      533.00000    LIQ        90.00                      .00000      .00000      .00000      .00000      .00000
                                                                  1.00000
         6     1978.45000    VAP        60.00                      .83000      .08400      .04800      .02600      .01200
                                                                   .00000
                    STAGE TEMPERATURES AND VAPOR FLOW RATES

                      USED TO INITIALIZE COLUMN ITERATIONS

                            TEMPERATURE         VAPOR RATE
                   STAGE     (DEG. F)          (LBMOLES/HR)
                   -----    ------------       ------------

                     1          80.00           1978.45000
                     2          94.00           1978.45000
                     3         108.00           1978.45000
                     4         122.00           1978.45000
                     5         136.00           1978.45000
                     6         150.00           1978.45000
INTERMEDIATE RESULTS WILL BE PRINTED OUT EVERY    2  COLUMN ITERATIONS

      AFTER ITERATION    1  CALCULATIONS ARE NOT CONVERGED.
      COLUMN ITERATION CONVERGENCE FACTOR IS      .88378+04  , WHICH IS GREATER THAN TOLERANCE OF    .06000



                          INTERMEDIATE RESULTS FOR ITERATION    2

        TEMP.     VAPOR RATE     LIQUID RATE    LIQUID, FOLLOWED BY VAPOR,MOLE FRACTIONS            LIQUID MOLE
STAGE  (DEG. F)  (LBMOLES/HR)   (LBMOLES/HR)     COMPONENTS 1 TO  6                                  FRACTION SUM
-----  --------  ------------   ------------   ----------------------------------------------------  ------------
  1     94.81     1889.02625      578.45999    .02709     .01216     .01810     .01649     .00147
                                               .88336
                                                                                                        .95868
                                               .84342     .00199     .04250     .01222     .00037
                                               .00010
  2     96.03     1934.48624      584.16192    .02613     .01209     .01951     .02172     .00303
                                               .85925
                                                                                                        .94172
                                               .82188     .08278     .04647     .01677     .00080
                                               .00010
  3     96.54     1940.18814      587.42429    .02612     .01215     .01982     .02461     .00509
                                               .85962
                                                                                                        .94742
                                               .81490     .08216     .04666     .01837     .00129
                                               .00010
  4     96.30     1943.45053      591.82612    .02672     .01254     .02042     .02822     .00855
                                               .87334
                                                                                                        .96980
                                               .81501     .08219     .04676     .01927     .00192
                                               .00009
  5     94.03     1947.85236      600.25410    .02782     .01318     .02130     .03440     .01601
                                               .89224
                                                                                                       1.00496
                                               .81904     .08265     .04708     .02034     .00296
                                               .00008
  6     85.95     1956.28035      622.42375    .02964     .01408     .02239     .04770     .03937
                                               .91072
                                                                                                       1.06390
                                               .82453     .08330     .04752     .02214     .00516
                                               .00006
          AFTER ITERATION    2  CALCULATIONS ARE NOT CONVERGED.
          COLUMN ITERATION CONVERGENCE FACTOR IS      .23435+03  , WHICH IS GREATER THAN TOLERANCE OF    .06000

          AFTER ITERATION    3  CALCULATIONS ARE NOT CONVERGED.
          COLUMN ITERATION CONVERGENCE FACTOR IS      .27976+01  , WHICH IS GREATER THAN TOLERANCE OF    .06000
```

```
                                  FINAL RESULTS

                       PRODUCT STREAMS AND EXCHANGER DUTIES

          FROM  PHASE      TEMP.      FLOW RATE       COMPONENT MOLE FRACTIONS
 STREAM   STAGE CONDITION (DEG. F)   (LBMOLES/HR)     FOR COMPONENTS 1 TO   6
 ------   ----- --------- --------   ------------   -------------------------------------------------------

GAS OUT     1     VAP       95.32     1889.47929     .85957    .08345    .04303    .01339    .00044
                                                     .00009
LIQ OUT     6     LIQ       85.48      621.97068     .02883    .01367    .02197    .04203    .03684
                                                     .85673
```

```
                                  FINAL RESULTS

                               INTERNAL CONDITIONS

                       FLOWS FROM STAGES
          TEMP.     VAPOR RATE    LIQUID RATE   LIQUID MOLE FRACTIONS                       VAPOR MOLE FRACTIONS
STAGE   (DEG. F)   (LBMOLES/HR)  (LBMOLES/HR)   COMPONENTS 1 TO   6                         COMPONENTS 1 TO   6
-----   --------   ------------  ------------   ----------------------------------------   ----------------------------------------

  1      95.32                    580.47253    .02827  .01279  .01885  .01986  .00199
                                               .91813
  2      96.87     1936.95181                                                              .84695  .08524  .04762  .01901  .00102
                                                                                           .00009
  2      96.87                    587.83845    .02767  .01294  .02071  .02745  .00447
                                               .90641
  3      97.42     1944.31775                                                              .84361  .08500  .04807  .02131  .00178
                                                                                           .00009
  3      97.42                    591.84126    .02749  .01287  .02084  .03047  .00768
                                               .90008
  4      96.90     1948.32056                                                              .84183  .08483  .04806  .02224  .00276
                                                                                           .00009
  4      96.90                    595.83775    .02750  .01288  .02089  .03209  .01205
                                               .89396
  5      94.09     1952.31705                                                              .84014  .08468  .04802  .02275  .00410
                                                                                           .00009
  5      94.09                    602.66273    .02778  .01306  .02116  .03447  .01913
                                               .88393
  6      85.48     1959.14204                                                              .83744  .08449  .04800  .02352  .00631
                                                                                           .00007
```

Comments on Sample-problem Results

For this relatively simple problem, convergence of the column iterations was rapid. Only four column iterations were required. An execution time of 1.8 seconds was needed to solve the problem on a Univac 1108 using Exec 8. This is equivalent to 0.45 second per column iteration.

The calculations indicate that the liquid product contains about 50% of the entering n-butane and almost all of the entering n-pentane. The vapor is heated from 60°F to 95°F in passing through the column, while the absorber oil cools from 90°F to 85°F. Very little of the absorber oil is stripped out into the vapor. An interesting student exercise is to plot the temperature, vapor/liquid traffic, and composition against stage number, using the final results. Also, it would be interesting to rerun the sample problem with a lower entering-oil temperature. Alternatively, the effect of adding an intercooler on the second stage could be studied.

CACHE COMPUTER PROGRAM

Program Name: LEACH
Class: Normal FORTRAN
Type: Self Standing

CACHE Number: VI-1
Date issued: 7-73

1. Title: Stagewise Leaching Process Calculations

2. Author: Harry G. Folster

3. Cognizant Supervisor: Harry G. Folster

4. Organization Name, Address, Telephone Number: Department of Chemical Engineering, New Mexico State University, Las Cruces, N.M. 88001, 505/646-2130.

5. Abstract: A description is given of a computer program which will determine the number of separation stages required to recover a specified quantity of $CuSO_4$ from roasted ore using water as the solvent. If the number of separation stages available are specified, the program will calculate the solvent rate required to obtain the specified recovery for a given feed rate and composition. The results, overall and stagewise material balances, are printed.

6. Related Programs: None

7. Program Development:
   - 7.1 Computer Used: IBM 1130
   - 7.2 Minimum Core: 8 K
   - 7.3 Operating Environment: Batch
   - 7.4 Language: FORTRAN IV
   - 7.5 Typical Run Time: 1-10 seconds
   - 7.6 No. of Source Cards: 132

CACHE COMPUTER PROGRAM

Program Name:

Class: (Normal or Limited FORTRAN)

Type: (Self-Standing or Subroutine(s) with Driver) Self-standing

CACHE Number: VI-2

Date Issued: 7-73

1. Title: (1 line) Optimum Stages in Leaching

2. Author(s): Ning Hsing Chen

3. Cognizant Supervisor:

4. Organization Name, Address and Telephone Number: Department of Chemical Engineering, Lowell Technological Institute, Lowell, Mass. 01854 617-454-7811 Ext. 340

5. Abstract: (20 line maximum)

Optimum theoretical stages, optimum solvent rate and hourly profit in leaching using the Newton Raphson method with the formulated economic objective function.

6. Related Programs:

7. Program Development:

7.1 Computer Used PDP-9

7.2 Minimum Core

7.3 Operating Environment Batch

7.4 Language FORTRAN IV

7.5 Typical Run Time about 6 seconds

7.6 No. of Source Cards

CACHE COMPUTER PROGRAM

Program Name: SOLIX
CACHE Number: VI-3
Class: Limited FORTRAN
Date Issued: 7-73
Type: Self-Standing

1. Title: Countercurrent Multi-Stage Solid-Liquid Extraction
2. Author: Charles M. Thatcher
3. Cognizant Supervisor: Charles M. Thatcher
4. Organization Name, Address and Telephone Number: Department of Chemical Engineering, University of Arkansas, Fayetteville, AR 72701
501-575-4951
5. Abstract:

The program uses the absorption-factor method to calculate the composition and quantity of all streams from input values of lb/hr of feed and solute mass fraction, lb/hr of solvent and solute mass fraction therein, solution/solids ratio in underflow streams, and number of equilibrium stages (N). N range is from 1 to 20, and any number of N values may be processed in a single run. The program does not provide for a limitation on solubility.

6. Related Programs: None
7. Program Development:

7.1 Computer Used	IBM 360 Model 50	7.4 Language	FORTRAN IV
7.2 Minimum Core	5,000 words	7.5 Typical Run Time	12 sec.
7.3 Operating Environment	Batch	7.6 No. of Source Cards	103

CACHE COMPUTER PROGRAM

Program Name: LIQLIQ
CACHE Number: VI-4
Class: Normal FORTRAN
Date Issued: 7-73
Type: Self-Standing

1. Title: Liquid-Liquid Extraction
2. Author: Edward C. Roche, Jr.
3. Cognizant Supervisor: Edward C. Roche, Jr.
4. Organization Name, Address, and Telephone Number:

Department of Chemical Engineering & Chemistry
Newark College of Engineering
323 High Street
Newark, New Jersey 07102

201-645-5394

5. Abstract:

The program input consists of the basic design data specifying the liquid-liquid extraction problem along with the associated equilibrium data in the form of the four suffix Margules equation constants. Starting with a set of internal flow rates and compositions for the extract and raffinate phases the stagewise problem is solved iteratively using the Newton Raphson algorithum until the conditions of stagewise material balance and equilibrium are satisfied. In addition, the program has the capabilities of handling as a design option problems involving extract reflux. Product specifications may be specified with the appropriate solvent feed stream rate being varied to obtain overall column convergence.

6. Related Programs: None

7. Program Development:

7.1 Computer Used: RCA3, Model 46
7.2 Minimum Core: 120K bytes
7.3 Operating Environment: Batch
7.4 Language: Fortran IV
7.5 Typical Run Time: 2 minutes
7.6 Number of Source Cards: 1366

CACHE COMPUTER PROGRAM

Program Name:
CACHE Number: VI-5
Class: (Normal or Limited FORTRAN)
Date Issued: 7-73
Type: (Self-Standing or Subroutine(s) with Driver)

1. Title: (1 line) Batch Distillation with Negligible Hold-up
2. Author(s): Jaime Wisniak - Armin Lauterbach
3. Cognizant Supervisor:
4. Organization Name, Address and Telephone Number: Department of Chemical Engineering, University of the Negev, Beer-Sheva, Israel
5. Abstract: (20 line maximum)
Batch distillation of a binary mixture with negligible hold-up, using constant or variable reflux.

6. Related Programs:
7. Program Development:

7.1 Computer Used IBM 360 Model 67
7.2 Minimum Core 16 K words
7.3 Operating Environment
7.4 Language FORTRAN IV
7.5 Typical Run Time Constant Reflux 5-10 min. Variable reflux 1-2 min.
7.6 No. of Source Cards 215

CACHE COMPUTER PROGRAM

Program Name: ______________________ CACHE Number: VI-6

Class: (Normal or Limited FORTRAN) Date Issued: 7-73

Type: (Self-Standing or Subroutine(s) with Driver) Self-standing

1. Title: (1 line) Continuous Multistage Binary Distillation
2. Author(s): Alkis Constantinides
3. Cognizant Supervisor: ______________________
4. Organization Name, Address and Telephone Number: Department of Chemical Engineering, Rutgers University, New Brunswick, N.J. 08903
   201-932-3678
5. Abstract: (20 line maximum)

   Performs stage-to-stage calculations for the distillation of a binary mixture. Uses material balances and equilibrium relations. Assumes constant molar overflow. The compositions of feed, distillate and bottoms are specified.

6. Related Programs: ______________________
7. Program Development:

   7.1 Computer Used IBM 360 Model 67

   7.2 Minimum Core 30K

   7.3 Operating Environment ~~Batch~~

   7.4 Language FORTRAN IV

   7.5 Typical Run Time 8 seconds

   7.6 No. of Source Cards 178

CACHE COMPUTER PROGRAM

CACHE Number: VI-7
Date issued: 7-73

Name: BATCH

Type: (Self-standing or Subroutine with Driver) Self-standing

1. Title: (1 line) Batch Distillation of Moonshine
2. Author(s): W. L. Luyben
3. Organization name, address and telephone number:
   Lehigh University, Bethlehem, Pa. 18015 (215-691-7000)
4. Abstract: (20 line maximum)

The dynamic changes in compositions over the course of a batch distillation are calculated by numerical integration of the ordinary differential equations describing the system.

5. Program Development:

5.1 Computer used: CDC 6400	5.2 Minimum core: 4 K
5.3 Operating environment: Batch	5.4 Language: FORTRAN IV
5.5 Typical run time: 7 sec.	5.6 No. of Source Cards: 59

CACHE COMPUTER PROGRAM

Program Name: __________ CACHE Number: VI-8

Class: (Normal or Limited FORTRAN) Date Issued: 7-73

Type: (Self-Standing or Subroutine(s) with Driver) Self-standing

1. Title: (1 line) Binary Distillation using McCabe-Thiele Assumptions
2. Author(s): John D. Stevens
3. Cognizant Supervisor: __________
4. Organization Name, Address and Telephone Number: Iowa State University, Chemical Engineering Department, Ames, Iowa 50010, 515-294-1660
5. Abstract: (20 line maximum)

A linear interpolation trial and error method is used to find the reflux ratio and bottoms composition in a binary distillation. The McCabe-Thiele method is used for stepping off ideal stages.

6. Related Programs: __________
7. Program Development:

7.1 Computer Used IBM 360 Model 65

7.2 Minimum Core 1000 words

7.3 Operating Environment Batch

7.4 Language FORTRAN IV

7.5 Typical Run Time 0.5 sec.

7.6 No. of Source Cards 59

CACHE COMPUTER PROGRAM

CACHE Number: VI-9
Date issued: 7-73

Name: Neil S. Berman

Type: Self - standing

1. Title: COMPO

2. Authors: Neil S. Berman and Joe McKee

3. Organization name, address and telephone number: Engineering Center Arizona State University, Tempe, Arizona 85281, 602-965-3836

4. Abstract:

This program tests a multicomponent distillation column to see if the desired separation is possible in the tested column. A Lewis-Matheson method with a linear initial temperature profile is used. The separation must have the heavy and light keys fixed in the distillate and bottoms, and the equilibrium constants must be available in the form of quadratic functions of temperature.

5. Program Development:

5.1 Computer used: CDC 6400
5.2 Minimum core: 8 K words
5.3 Operating environment: Batch
5.4 Language: FORTRAN IV
5.5 Typical run time: 7 seconds
5.6 No. of Source Cards: 170

CACHE COMPUTER PROGRAM

CACHE Number: VI-10
Date issued: 7-73

Name: Orville C. Sandall

Type: (Self-standing or Subroutine with Driver) Self-standing

1. Title: MLTCOMP

2. Author: Orville C. Sandall

3. Organization name, address and telephone number: (805) 961-2908
Department of Chemical and Nuclear Engineering
University of California, Santa Barbara, Calif. 93106

4. Abstract:

Stage-to-stage calculations based on the Lewis-Matheson method are performed in connection with the design of a distillation column to separate a four component hydrocarbon mixture. It is assumed that the vapor-liquid equilibrium may be described by a constant relative volatility. The technique of Bonner is used to adjust product distributions in order to achieve a feed plate match.

5. Program Development:

5.1 Computer used: IBM 360/75
5.2 Minimum core: 40 K BYTES
5.3 Operating environment: Batch
5.4 Language: FORTRAN IV
5.5 Typical run time: 6.90 sec.
5.6 No. of Source Cards: 102

CACHE COMPUTER PROGRAM

CACHE Number: VI-11
Date issued: 7-73

Name: DONALD MACKAY

Type: (Self-standing or Subroutine with Driver) Self-standing

1. Title: (1 line) Multicomponent Distillation

2. Author(s): Donald Mackay

3. Organization name, address and telephone number: Department of Chemical Engineering and Applied Chemistry, University of Toronto, Toronto 181, Ontario, 416-928-3060.

4. Abstract: (20 line maximum)

The program computes the distillate and bottoms composition resulting from a specified distillation column with specified multicomponent feed and reflux ratio. A Lewis and Matheson plate-to-plate method with theta convergence is used. By trial and error columns meeting required separation specifications can be found and costed.

5. Program Development:

5.1 Computer used: IBM 370
5.2 Minimum core: 13 K
5.3 Operating environment: Self-serve
5.4 Language: Fortran IV
5.5 Typical run time: 2 Second
5.6 No. of Source Cards: 257

CACHE COMPUTER PROGRAM

CACHE Number: VI-12
Date issued: 7-73

Name: David M. Watt, Jr.
Type: Self-standing

1. Title: Multicomponent Distillation--Design Case
2. Authors: Jean P. Leinroth, Jr. and David M. Watt, Jr. (at Cornell University during the development of the problem).
3. Organization name, address and telephone number: Procter & Gamble Co., Miami Valley Laboratories, P. O. Box 39175, Cincinnati, Ohio 45239, 513-738-1111.
4. Abstract:

For a multicomponent bubble point feed of known composition, this program calculates down tray-by-tray from the total condenser with specified distillate composition until the ratio of the mole fractions of the light and heavy keys is less than the corresponding ratio in the feed. This gives the number of trays above the feed. Similar tray-by-tray calculations from the reboiler with specified bottoms composition up the column until the ratio of the mole fractions of the light and heavy keys is greater than the corresponding ratio in the feed gives the number of trays below the feed. This calculation gives the total number of required trays for the separation, but it leaves a composition discontinuity at the feed tray. This design number of required trays can then be used in a column rating calculation to determine the actual distillate and bottoms compositions. (See CACHE problem "Multicomponent Distillation-Rating Case.)

Antoine constants are calculated from vapor pressure data, and Raoult's law is used to calculate vapor-liquid equilibrium constants. Constant molal overflow is assumed. Dew point and bubble point subroutines use the Newton-Raphson method and were developed for CACHE problem "Bubble and Dew Point Calculations with Ideal Mixtures."

CACHE COMPUTER PROGRAM

Name: David M. Watt, Jr.

CACHE Number: VI-13

Date issued: 7-73

Type: Self-standing

1. Title: Multicomponent Distillation--Rating Case

2. Authors: Jean P. Leinroth, Jr., and David M. Watt, Jr., (at Cornell University during the development of the problem)

3. Organization name, address and telephone number:
Procter & Gamble, P. O. Box 39175, Cincinnati, Ohio 45239
513-738-1111

4. Abstract:

For a multicomponent liquid feed to a specified distillation column, the exact distillate and bottoms compositions are calculated using the Thiele-Geddes iterative technique. Bubble point and dew point subroutines were developed for CACHE problem "Bubble and Dew Point Calculations with Ideal Mixtures" and are used with this program. The number of ideal stages required above and below the feed can be found with the CACHE program "Multicomponent Distillation--Design Case." This "Design Case" program is the basis for building the "Rating Case" program and enables the student to complete the problem in a single assignment.

In this iterative method calculations proceed from an estimate of the distillate composition down to the feed tray and from an estimate of the bottoms composition up to the feed tray. The ratio of these two calculated feed tray compositions is used to improve the estimates of the distillate and bottoms compositions. About ten iterations are usually sufficient for satisfactory convergence.

CACHE COMPUTER PROGRAM

Program Name: ______ CACHE Number: VI-14

Class: (Normal or Limited FORTRAN) ______ Date Issued: 7-73

Type: (Self-Standing or Subroutine(s) with Driver) Self-standing

1. Title: (1 line) Equilibrium Separation in a Multicomponent Multicolumn System
2. Author(s): John W. Tierney
3. Cognizant Supervisor: ______
4. Organization Name, Address and Telephone Number: University of Pittsburgh Department of Chemical Engineering, 15213 412-621-3500
5. Abstract: (20 line maximum)
A program to solve for temperatures and stage compositions in a multicomponent multicolumn distillation system. Flow rates are known and are not changed. Heat balancing is not included.

6. Related Programs: ______
7. Program Development:

7.1 Computer Used IBM 360-50

7.2 Minimum Core 8,000

7.3 Operating Environment Batch

7.4 Language FORTRAN IV

7.5 Typical Run Time 1 minute

7.6 No. of Source Cards 210

CACHE COMPUTER PROGRAM

Program Name:		CACHE Number:	VI-15
Class: (Normal or Limited FORTRAN)		Date Issued:	7-73

Type: (Self-Standing or Subroutine(s) with Driver) Silf-standing

1. Title: (1 line) Amundsen-Pontinen Distillation
2. Author(s): L. L. Hovey
3. Cognizant Supervisor:
4. Organization Name, Address and Telephone Number: Department of Chemical Engineering, University of Wyoming, Laramie, Wyoming 82070

   307-766-3170
5. Abstract: (20 line maximum)

A tray to tray multicomponent distillation program using the Amundsen-Pontinen method of solution. Up to 12 components and 48 trays plus a reboiler are permissible. Raoult's law is used for "K" values. Average heats of vaporization and liquid heat capacities are used for enthalpy balances. Overhead, bottoms, and tray compositions are calculated per 100 moles of feed, given feed composition, overhead rate, bottoms rate, vapor rate to the condenser, total stages, number stages below the feed stage, number of components, overhead pressure, pressure drop per tray, feed temperature and feed enthalpy references to liquid at 0°F. Vapor pressure data in the form $\mathrm{Ln}\ (P) = A + B/T + C/T^2$ where P is in mm Hg and T is °K is also required.

6. Related Programs:
7. Program Development:

7.1 Computer Used	XDS Sigma 7	7.4 Language	FORTRAN IV
7.2 Minimum Core	7500 words	7.5 Typical Run Time	12 seconds
7.3 Operating Environment	Batch	7.6 No. of Source Cards	290

CACHE COMPUTER PROGRAM

Program Name: WHENDI
CACHE Number: VI-16

Class: Normal F0RTRAN
Date Issued: 7-73

Type: Subroutines with Driver

1. Title: Multicomponent Distillation by the Wang-Henke Method

2. Authors: P. J. Johansen and J. D. Seader

3. Cognizant Supervisor: Professor J. D. Seader

4. Organization Name, Address, and Telephone Number:

Chemical Engineering Department
The University of Utah
Salt Lake City, Utah 84112

(801) 581-6585

5. Abstract:

WHENDI can be used to solve a wide variety of multicomponent distillation problems by rigorous material and energy balances around each theoretical stage. Feeds, liquid and vapor sidestreams, and heat transfer to or from any interior stage can be specified. The program is limited to a maximum of 100 theoretical stages and 20 chemical species. K-value and enthalpy data for each species are computed from polynomial equations in temperature. The user must supply the coefficients of polynomial equations for the specified distillation pressure.

Important features of the Wang-Henke method used in the program are solution of the linearized material-balance equations by a tridiagonal matrix method and solution of the nonlinear bubble-point equations by Muller's iterative scheme. The program provides a convenient printout of input data and results. Error messages are included to guide the user in overcoming any difficulties. WHENDI should not be used for absorbers, strippers, reboiled absorbers, etc.

6. Related Programs: FLASHC, STAB

7. Program Development:

7.1 Computer Used: Univac 1108

7.2 Minimum Core:

	Inst	Data
Main	1172	1556
Subprograms	915	614
Common	0	21357
System	4051	195
Total	6138	23722

Combined Total: 29860

7.3 Operating Environment: Batch with Exec 8 system

7.4 Language: F0RTRAN-IV

7.5 Typical Run: 5.6 seconds for Sample Problem

7.6 No. of Source Cards: 635

CACHE COMPUTER PROGRAM

Program Name: STAB
CACHE Number: VI-17
Class: Normal FØRTRAN
Date Issued: 7-73
Type: Subroutines with Driver

1. Title: Multicomponent Stripping and Absorption

2. Authors: T. Shinohara, P. J. Johansen, and J. D. Seader

3. Cognizant Supervisor: Professor J. D. Seader

4. Organization Name, Address, and Telephone Number:

   Chemical Engineering Department
   The University of Utah
   Salt Lake City, Utah 84112

   (801) 581-6585

5. Abstract:

STAB can be used to solve a wide variety of multicomponent stripping and absorption problems by rigorous material and energy balances around each theoretical stage. Feeds, liquid and vapor side-streams, and heat transfer to or from any stage can be specified. The program is limited to a maximum of 100 theoretical stages and 20 chemical species. K-value and enthalpy data for each species are computed from polynomial equations in temperature. The user must supply the coefficients of the polynomial equations for the specified operating pressure.

The program is based on an extension of the Wang-Henke method by Burningham and Otto. Important features include solution of the linearized material-balance equations by a tridiagonal matrix method and solution of the heat-balance equations for stage temperatures by the Newton-Raphson method. STAB is not intended for application to distillation or reboiled-absorption calculations.

6. Related Programs: WHENDI

7. Program Development:

7.1 Computer Used: Univac 1108

7.2 Minimum Core:

	Inst	Data
Main	1075	1358
Subprograms	1096	738
Common	0	31404
System	4018	2233
Total	6189	35733

Combined Total: 41922

7.3 Operating Environment: Batch with Exec 8 System

7.4 Language: FØRTRAN-IV

7.5 Typical Run: 1.8 seconds for Sample Problem

7.6 No. of Source Cards: 592